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Extending scaling analysis of the Ising Model

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Extended Scaling Analysis

of the

Ising Model

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Summary

Phase transitions play an important role in the field of statistical mechanics and such phenomena are manifest in everyday life. Examples include the evaporation of water, magnetisation of metals and the jamming of traffic. The purpose of this project is to examine the properties of phase transitions in the model of magnets known as the Ising model and to test a recent approach (extended scaling) to their analysis. The literature is abundant with many models which describe phase transitions; with the Ising model being the one which is most broadly studied (approximately 700-900 papers are published each year, which have some relationship to the Ising model). The first objective is to analyse the Ising model as an example of a mathematical model of phase transitions. In particular, the exact solution of the Ising model in one dimension is derived and the mean field approach is also considered. The scaling behaviour of these Ising models is examined in the context of the scaling relations which are also derived.

Since no exact solution is available, approximate methods must be used to investigate the phase transition of the Ising model in higher dimensions. In particular, one is interested in the scaling behaviour of various thermodynamic functions close to the phase transition. One such method is the high-temperature series expansion. A new method has recently been proposed to extract the scaling behaviour, which is claimed to be superior to the traditional approach. This so-called extended scaling approach has been tested only in two and three dimensions at temperatures above the phase transition.

Here, the new scheme is retested in two dimensions to gain experience in the technique. It is then applied and tested for the first time above the upper critical dimension. It is demonstrated to be successful there in the sense that it follows the critical expansion in the critical regime and follows the high temperature series expansion in the high temperature regime.

The application of this new technique in high dimensions led on to a jointly authored paper which has now been published (Appendix D).

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Abstract

Properties of phase transitions are investigated in the Ising model in various dimensions. The re-derivation of the exact solutions of one and infinite-dimensional models using the transfer matrix technique and the mean field method is presented. The scaling behaviour of these Ising models is examined in the context of the scaling relations which are also derived. The recently proposed extended scaling method to extract scaling behaviour, which is claimed to be superior to the conventional approach, was retested in the two-dimensional Ising model to gain experience. It is then applied and tested in an analysis of the magnetic susceptibility of the Ising systems above the upper critical dimension, four. It is seen that the extended scaling method broadens the high-temperature critical scaling regime to a range of temperatures much wider than that achieved traditionally, and is demonstrated to be applicable in high dimensions.

1 Introduction

Statistical Mechanics has proven to be an extremely important area of science and mathematics. Phase transitions and critical phenomena are two aspects of statistical mechanics and are of central interest to this research. Phase transitions in general can be seen in everyday life, for instance, the transitions between solid, liquid and gaseous state and the traffic congestion. The central aim of this project is to examine the properties of the phase transitions in the Ising model in various dimensions.

The Ising model is an example of a model of a magnet which helps in analyzing the systems which undergo phase transitions. A sample of iron which is usually referred as a ferromagnet, for example, can be magnetized at room temperature. However, at and above certain temperature, known as critical temperature, the magnet losses its magnetic properties and becomes demagnetised. I.e, the system changes its phase from ferromagnetic to paramagnetic. While in day-to-day life ones experience is with magnets in three dimensions, the mathematical Ising model allows for consideration of magnetisation in any number of dimensions.

Inspired and guided by W. Lenz, in 1922 E. Ising created a landmark in the history of physics by solving the model in d=1 dimension and established that no phase transition occurs at finite temperature. In 1944, L. Onsager established the occurrence of phase transitions in the two-dimensional version of the model, which he solved in the absence of an external magnetic field. To this day, no accepted exact solution exists in two dimensions in field, or in three or higher dimensions. The mean-field version of the model has, however, been exactly solved and is applicable to infinite-dimensional space.

In the first part of this project, experience in the Ising model is gained by rederiving the exact solutions given for one-dimensional and mean field theory. Since, the first two objectives involve re-deriving the solution of Ising model in one-dimension and infinite dimensions (mean field theory) they involve not only advanced mathematics (drawing on

calculus, algebra and various statistical-mechanical concepts) but also involves theoretical knowledge of statistical mechanics. The emphasis in the first part of the project, therefore, lies with the analytical approach as used in previous studies for the exact solutions. In particular, the transfer matrix technique is used for $d = 1$ and the Bragg-Williams approach, Weiss Mean Field and the saddle point solution gives the Ising model in infinite dimensions.

The second and principle part of the project involves an investigation into the scaling behaviour of the Ising model in high dimensions, with d=5, 6, 7 and 8 being targeted. To gain experience, the analyses proposed recently will first be reproduced in d=2 dimensions. Subsequently, high-temperature series expansions in 5, 6, 7 and 8 dimensions will be analysed using traditional and extended scaling approaches with a view to comparing their applicability. This original research will involve a approach where the expansions for the magnetic susceptibility will be used. Since these expansions are to fifteenth order in the inverse temperature, the symbolic manipulation package MAPLE is used.

Thus, the central aim of this work is to present a first investigation of the efficacy of the extended scaling approach in high dimensions. In the following chapter, statistical mechanics is introduced and then the phase transitions are discussed in generally. In chapter 3, the Ising model is presented together with a brief discussion of its history. Types of phase transitions and the other models in Statistical mechanics are discussed in chapter five and six, respectively. Scaling relations are determined in chapter 7. The exact solution to the one-dimensional Ising model and it mean field version are presented in chapter 8 and 9. Finally, the extended scaling is introduced in chapter 10 and applied to the Ising model in $d = 2$ dimension and the above the upper critical dimension $d = 4$.

2 Statistical Mechanics

According to the Dalton atomic theory of 1803, "matter is made up of very tiny particles called atoms" (Dalton 1805). This means that even a small sample of some material will be composed of a very large number of such tiny particles. The number of particles is of the order of Avogadro's number $N_A = (6.022\,141\,79 \pm 0.000\,000\,30) \times 10^{23}$. Because of this it is impossible to determine the properties of the full system by tracking the behaviour of the individual particles. Instead a statistical approach must be used. The field of statistical mechanics aims to make a connection between the macroscopic and microscopic properties of the system by statistically relating the properties of the whole system with the properties of its individual particles (see, e.g., Glazer and Wark (2006)).

Statistical mechanics has proven to be an extremely important area of science, mathematics and engineering in addressing many diverse problems (see e.g., Ruelle (1988)). Furthermore, statistical-mechanics concepts and methods are widely used in various other different areas such as dynamical systems, turbulence, communications, quantum field theory, finance and bioinformatics. Statistical mechanics was developed by Willard Gibbs and others in the middle of nineteenth century as a way to study the influence of micro physics on the macroscopic properties of matter. This development of statistical mechanics explains thermodynamics (which deals only with the large-scale properties) at a microscopic level i.e, relating the thermodynamic properties of a large system with the individual atoms and molecules. Thus, the microstates of the system gives the detailed specification of all the particles in a system, i.e., the properties of the system are determined by its microstates. On the other side, the macroscopic picture only gives the essential information which are required for the description of any system, i.e., it is a description of the thermodynamic variables: energy, volume, pressure, temperature and magnetisation. As a result, it can be said that large number Ω of microstates correspond to single macrostate of the system i.e, determining the individual particles in the system, the thermodynamic properties of the large system can be found.

The fundamental postulate of statistical mechanics is stated as "all possible microstates of an isolated assembly are equally probable." This postulate implies that the most probable macrostate is the one with the largest number of microstates.

Next, in order to justify this assumption consider N distinguishable particles associated with the energies $\epsilon_1, \epsilon_2, \cdots, \epsilon_j, \cdots$ and the given macrostates of the system are the total internal energy U and the volume V. Thus, a given distribution should follow

$$\begin{aligned} n_1 \quad &\text{particles with an energy} \quad \epsilon_1 \\ n_2 \quad &\text{particles with an energy} \quad \epsilon_2 \\ &\vdots \\ n_j \quad &\text{particles with an energy} \quad \epsilon_j \\ &\vdots \end{aligned} \tag{2.1}$$

Therefore, the number of particles is

$$N = \sum_j n_j, \tag{2.2}$$

and the total internal energy which is the sum of the individual energies of the distribution is then

$$U = \sum_j n_j \epsilon_j. \tag{2.3}$$

The number of microstates for the above given distribution is the number of ways in which N object can be divided into piles with n_1 in the first pile, n_2 in the second pile, etc. This is

$$t = \frac{N!}{n_1!, n_2! \cdots n_j! \cdots}. \tag{2.4}$$

A different distribution will have different values for $n_1, n_2, \cdots$. The total number of microstates Ω is

$$\Omega = \sum_{\text{distributions}} t = \sum_{n_1, n_2, \cdots} \frac{N!}{n_1!, n_2! \cdots n_j! \cdots}. \tag{2.5}$$

Next, in order to demonstrate this, consider an assembly of three distinguishable particles, A, B and C where each particle is assumed to have any energy from $\epsilon_0 = 0, \epsilon_1 = \epsilon, \epsilon_2 =$

$2\epsilon \cdots \epsilon_j = j\epsilon$. Suppose, the total internal energy is fixed by

$$U = 3\epsilon. \tag{2.6}$$

There exist only three possible ways in which the internal energy can be divided among the three particles. These three distributions I, II and III, are

I	ϵ	ϵ	ϵ
II	3ϵ	0	0
III	2ϵ	ϵ	0

In the first distribution each particle has energy ϵ, so $n_0 = n_2 = n_3 = 0$ and $n_1 = 3$. As a result, from (2.4), the number of microstate for this distribution is

$$t(1) = \frac{3!}{3!0!0!0!} = 1. \tag{2.7}$$

Similarly, the number of possible microstates for the other distributions is given by (2.4). As a result, the second and third distribution have 3 and 6 microstates. From (2.5), the total number of microstates is $\Omega = 10$. Table 2.1 shows the arrangement of all these possible 10 microstates. As each column indicates one microstate, therefore, there are 10 microstates which are all equally probable for this assembly.

Table 2.1

A	ε	3ε	0	0	2ε	2ε	ε	ε	0	0
B	ε	0	3ε	0	ε	0	2ε	0	2ε	ε
C	ε	0	0	3ε	0	ε	0	2ε	ε	2ε
		I		II			III			

It can be seen from table 2.1 that the most probable distribution is the third one because it occurs 6 times. Therefore, the maximum value of t is

$$t_{\max} = 6. \tag{2.8}$$

When large numbers of particles are involved, it turns out (Guenault 2007) that the most probable distribution is overwhelmingly more probable than the others i.e., the function t has a sharp peak. Therefore, instead of considering all the distributions, the results can be found by simply choosing the most probable distribution. From (2.4) and (2.5), the microstate Ω is

$$\Omega \simeq t_{\max} \tag{2.9}$$

Now maximize Ω subject to two conditions (2.2) and (2.3). At maximum

$$d\Omega = 0. \tag{2.10}$$

Since

$$d(\ln \Omega) = \frac{1}{\Omega} d\Omega = 0. \tag{2.11}$$

Therefore, $\ln \Omega$ can be maximized instead of Ω.

Next, for any small change in $n_1, n_2 \cdots$, the change in $\ln \Omega$ is

$$d \ln \Omega = \frac{\partial \ln \Omega}{\partial n_1} dn_1 + \frac{\partial \ln \Omega}{\partial n_2} dn_2 + \cdots. \tag{2.12}$$

and the above expression equals zero for the $\ln \Omega$ maximum. Since N and U in (2.2) and (2.3) are fixed,

$$dN = \sum_j dn_j = 0, \tag{2.13}$$

and

$$dU = \sum_j \epsilon_j dn_j = 0. \tag{2.14}$$

Thus the problem is one of maximization subject to contraint. Multiplying (2.13) by α and (2.14) by $-\beta$, where α and β are Langrange multipliers, and then adding both to (2.12) gives

$$\sum_j \left[\frac{\partial \ln \Omega}{\partial n_j} + \alpha - \beta \epsilon_j \right] dn_j = 0. \tag{2.15}$$

Since the particles in the above formulation are independent of each other therefore, one can consider

$$\frac{\partial \ln \Omega}{\partial n_j} + \alpha - \beta \epsilon_j = 0. \tag{2.16}$$

Using the Stirling Approximation, expression (2.9) can be written as

$$\begin{aligned} \ln \Omega &= \ln \frac{N!}{n_1! n_2! \cdots n_j! \cdots}, \\ &= \ln N! - \sum_j \ln n_j!, \\ &= \ln N! - \sum_j (n_j \ln n_j - n_j). \end{aligned} \tag{2.17}$$

Differentiating the above expression gives

$$\frac{\partial \ln \Omega}{\partial n_j} = -\frac{\partial}{\partial n_j}(n_j \ln n_j - n_j),$$

$$\frac{\partial \ln \Omega}{\partial n_j} = -\ln n_j. \tag{2.18}$$

Substituting the above result in (2.16) gives

$$-\ln n_j + \alpha - \beta \epsilon_j = 0. \tag{2.19}$$

which can be equivalently written as

$$n_j = e^{\alpha} e^{-\beta \epsilon_j}. \tag{2.20}$$

Now substituting the value for n_j in (2.2) gives

$$N = e^{\alpha} \sum_j e^{-\beta \epsilon_j}, \tag{2.21}$$

Rearranging above for α gives

$$e^{\alpha} = \frac{N}{\sum_j e^{-\beta \epsilon_j}}. \tag{2.22}$$

Let $Z = \sum_j e^{-\beta \epsilon_j}$. Then

$$n_j = \frac{N}{Z} e^{-\beta \epsilon_j}. \tag{2.23}$$

This scheme is called the Boltzmann distribution. The normalization factor Z is known as the partition function, which will be important subsequently.

Next, substituting (2.23) into (2.3) gives

$$U = \frac{N}{Z} \sum_j \epsilon_j e^{-\beta \epsilon_j}. \tag{2.24}$$

The internal energy per particle is

$$\frac{U}{N} = \frac{1}{Z}\sum_j \epsilon_j e^{-\beta\epsilon_j}. \tag{2.25}$$

which is the expectation value taken over the Boltzmann distribution.

It turns out that β can be identified as proportional to the inverse absolute temperature.

$$\beta = \frac{1}{kT}. \tag{2.26}$$

where k is the Boltzmanns constant whose value is $1.3807 \times 10^{-23} JK^{-1}$.

3 Phase Transitions

Defining Phase Transitions

Phase transitions play important roles in the field of statistical mechanics and such phenomena are manifest in many day to day experiences, for example, melting of ice and evaporation of water. Moreover, scientifically, one can describe a phase transition as a transmutation of a thermodynamic system from one phase to another. For example, transitions between solid, liquid, and gaseous states of matter. Water at room temperature is in liquid form. If the temperature is sufficiently reduced, the liquid forms into ice (solid) and if the temperature is sufficiently increased then water changes into steam or vapour (gas). This transition is possible due to change in either temperature or pressure of the system or both. This is an example of a liquid-gas-solid transition and is illustrated in figure 3.1.

Figure 3.1: Phase transitions of water (Dobrosavljevic 2005)

This figure represents the pressure and temperature graph where coexistence of all the three states (gas, liquid and solid) occur at one point known as the triple point. Also, when both temperature and pressure increases, it reaches at a stage where liquid as well as gas are in an equilibrium state. This state is known as supercritical fluid (Poliakoff

2001). The point where there is a change in phase from one to another is known as the critical point, a notion introduced by Andrews (1869).

Non-Equilibrium Transitions: Besides water, another common example of phase transition can involve traffic congestion. Traffic may be in a free-flowing phase or in a congested (stationary) phase. Between them is another phase transition. A reduction in symmetry is associated with such a phase transition. In the example of traffic congestion, when a number of vehicles are clustered together, the system possesses fewer symmetrical properties compared to the vehicles moving smoothly where the system is more symmetrical. I.e, the smooth flow of traffic is associated with a higher degree of symmetry than the congestion in traffic. A more familiar example of a phase transition in statistical physics is magnetisation, discussed in the next paragraph.

Ferromagnetism

A sample of iron, for example, can be magnetized at room temperature. This common type of a magnet is usually called a ferromagnet. From a molecular point of view any ferromagnetic material shows the phenomenon of long range ordering, which means that the inherent molecules exist in aligned sets of domains. There is also a possibility for these sets of domains to be unaligned, however, an external field can force these domains to become aligned and consequently show magnetic properties (Nave 2006). It is important to note that one common property of any ferromagnet, be it iron or nickel or gadolinium, is that they all lose their magnetic properties at and above a certain temperature known as the critical temperature, T_c. Thus, above the critical temperature this substance can be described as paramagnetic. The change in magnetic properties between the paramagnetic phase and ferromagnetic phase is a phase transition. Figure 3.2 exhibits this behaviour and also shows that on an increase in temperature, the system's magnetism keeps decreasing until the temperature T_c is reached. At any temperature beyond T_c the system is demagnetised.

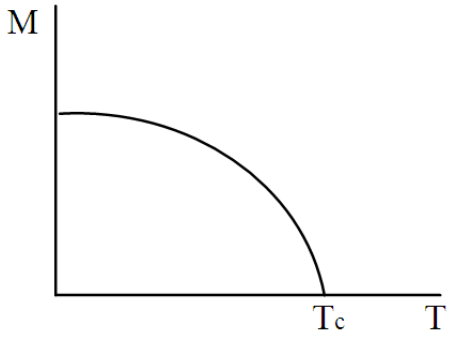

Figure 3.2: Phase transition of a magnet

At a point where the system's temperature is just less than the critical temperature T_c, the magnetic strength can usually be mathematically described as

$$m \sim |T_c - T|^{\beta} \quad \text{for} \quad T < T_c. \tag{3.1}$$

where β is a critical exponent. This statement is a result of empirical observation. A critical exponent, first introduced by Verschaffelt (1900), describes the behaviour of the system near the critical temperature. Critical exponents depend upon the dimension of both the system and spins as well as on the range of interaction. Now, in order to describe the thermodynamic quantities near the critical temperature, the reduced temperature, t, is introduced. The standard reduced temperature is defined as

$$t = \frac{T - T_c}{T_c}. \tag{3.2}$$

The Ferromagnetic behaviour can also be written in terms of the reduced temperature as

$$m \sim \begin{cases} |t|^{\beta} & \text{for } t < 0 \\ 0 & \text{for } t > 0 \end{cases} \tag{3.3}$$

The system is in an ordered phase when the system's magnetisation is non-zero and is in a disordered phase when the magnetisation is zero. Thus, this thermodynamic quantity, magnetisation discriminates the phase. For this reason it is known as an order parameter.

4 Ising Model

The Ising model is one of the most renowned in statistical mechanics. It exhibits the behaviour of a simple magnet near the critical temperature. As the temperature increases the system loses it magnetic properties and becomes demagnetised, as shown in figure 3.2. While in day-to-day life one's experience is with magnets in three dimensions, the mathematical Ising model allows for consideration of magnetisation in any number of dimensions. In this project the cases of the one-dimensional and mean field Ising model are considered.

Description

At a microscopic level, a piece of iron, for example, may be considered to be made up of spins, each with its own south and north poles. In figure 4.1, the spins are represented using arrows which are pointing in random direction.

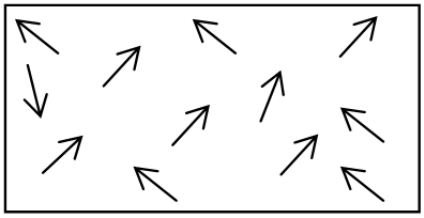

Figure 4.1: Microscopic image of a magnet

Now, the spins may be restricted to point in a particular direction, as shown in figure 4.2, where they only point upward or downwards. Furthermore, the spins are placed on a lattice of N sites, each site labelled by $i = 1, 2 \cdots, N$. If there are L sites in each of the d dimensions then

$$N = L^d. \tag{4.1}$$

The spin s_i at each site i has two possible values, given by ± 1, indicating the spins in an upward direction when s_i has a value of $+1$ and in a downward direction at a value -1.

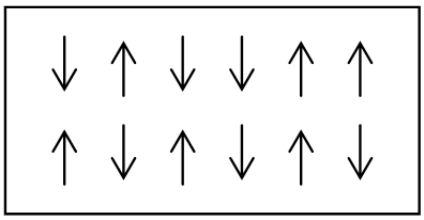

Figure 4.2: Spins restricted to a regular lattice

On a lattice, at high temperature these spins do not direct themselves to any particular direction and makes the piece of iron symmetric. On the other hand, at low temperature, which is usually referred as a '*broken phase*', the spins align themselves in one direction either in southwards or northwards. This disturbs the inherent symmetry of the system. The energy of the system is associated with the interaction between the spins. Consequently, the parallel spins result in a relatively low energy i.e., $-J$ whereas others result in a relatively higher energy i.e., J. Therefore, the energy related to the spins, s_i and s_j may be defined as

$$E = -Js_is_j, \tag{4.2}$$

where J is the interaction strength. In this scenario every spin is just allowed to interact with only the nearby neighbours, as shown in figure 4.3. Thus, the energy can now be defined as

$$E = -J \sum_{<i,j>} s_is_j. \tag{4.3}$$

where the summation is over all the nearest neighbours i and j.

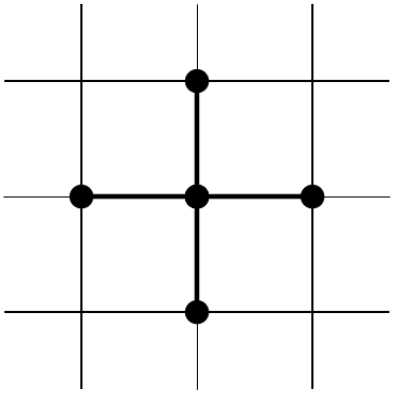

Figure 4.3: A representation of the nearest neighbours on a lattice.

It is important to note that there are many patterns in which the spins can be configured and as the number of spins are increased then automatically the number of ways to arrange the spins also increases. Since, each spin has two possible directions to point in and in a system there are N sites, therefore, there are 2^N configurations. Three such possible arrangement of spins are illustrated in figure 4.4, where each arrangement has four spins pointing up and two pointing down. Even though all the three arrangements have almost the same outlook, however, they have different microscopic characteristics.

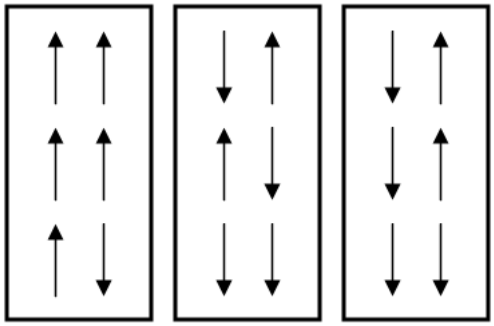

Figure 4.4: Possible arrangements of spins

Now, an external magnetic field is introduced to the system. This interacts with each spin in the system and the associated energy is given by

$$-\sum_i Hs_i. \tag{4.4}$$

From (4.3) and (4.4) the total energy of the system E_T, in the presence of external field is given by

$$E_T = -J \sum_{\langle i,j \rangle = 1}^{N} s_i s_j - H \sum_{i=1}^{N} s_i. \tag{4.5}$$

Now, the total magnetisation M of a configuration is the sum of the spins;

$$M = \sum_{i=1}^{N} s_i. \tag{4.6}$$

Therefore, the total energy may be written as

$$E_T = E - HM. \tag{4.7}$$

From the theory of Statistical Mechanics, the magnetisation of the system can be defined as a weighted average of the configurational magnetisation (Binney *et al.* 2002) i.e,

$$m = \frac{1}{N}\langle M \rangle = \frac{1}{N} \sum_{i} \langle s_i \rangle. \tag{4.8}$$

where M is defined in (4.6). Assuming translational invariance (the question of boundary conditions will be discussed at the end of this section), $\langle s_i \rangle$ is independent of i. Then the magnetisation is given by

$$m = \langle s_i \rangle, \tag{4.9}$$

$$= \frac{1}{Z} \sum_{\{s_i\}} s_i e^{-\frac{1}{kT} E_T}. \tag{4.10}$$

where k is the Boltzmann constant and the sum is taken over the configurations. The normalization factor Z is known as the partition function and is defined in terms of temperature and the external field as

$$Z(T, H) = \sum_{\{s_i\}} e^{-\beta E_T}. \tag{4.11}$$

Here

$$\beta = \frac{1}{kT}, \tag{4.12}$$

Next, introduce the reduced external field as

$$h = \beta H. \tag{4.13}$$

The expression for the partition function can now be expressed as

$$Z(\beta, h) = \sum_{\{s_i\}} e^{-\beta E + hM}. \tag{4.14}$$

Another important thermodynamic quantity in statistical mechanics is the free energy per particle f, which is simply derived by taking the partition function's logarithm:

$$f = \frac{-kT}{N} \ln Z(\beta, h). \tag{4.15}$$

Thermodynamic Functions

In thermodynamics, magnetisation, magnetic susceptibility, internal energy and specific heat are thermodynamic functions that can be derived from the partition function. These quantities react to the effects in the change of external conditions i.e. temperature T and external field H. In Appendix A, it is shown that the magnetisation is the first derivative of the free energy with respect to H;

$$m = -\frac{\partial f}{\partial H}. \tag{4.16}$$

The magnetic susceptibility, denoted by χ, is defined as the variance of the total magnetisation of all the spins, which can be written as

$$\chi = \frac{1}{N} \langle (\langle M \rangle - M)^2 \rangle. \tag{4.17}$$

and from the definition of total magnetisation (4.6), this can be equivalently written as

$$\chi = \langle (s_i - \langle s_i \rangle)^2 \rangle. \tag{4.18}$$

(provided the system is translationally invariant). Also, susceptibility is the second derivative of the free energy in terms of reduced external field (Ravndal 1976) and is denoted by

$$\chi = \frac{\partial^2 f}{\partial h^2}. \tag{4.19}$$

This relation has been derived in Appendix A.

The internal energy is defined as the expectation value of the energy and also can be expressed as the first derivative of the free energy, with respect to β. Its derivation is given in Appendix A and is denoted by

$$e = \frac{\partial f}{\partial \beta} = \frac{1}{N}\langle E \rangle. \tag{4.20}$$

Finally, the specific heat C is defined as the variance of the energies. This can also be expressed using the free energy i.e, differentiating twice the free energy with respect to β gives the specific heat as

$$C(\beta, h) = \frac{\partial^2 f}{\partial \beta^2} = \frac{1}{N}\langle (\langle E \rangle - E)^2 \rangle. \tag{4.21}$$

The derivation of the above relation has been given in Appendix A. This term can also be rewritten in terms of temperature by using the definition of β. Thus, again differentiating twice the free energy with respect to temperature yields

$$C = -T\frac{\partial^2 f}{\partial T^2}. \tag{4.22}$$

These derivations of all the thermodynamic variables reveal changes in a system brought by the change in temperature and external magnetic field. This also forms the basis for further calculations involved in the later sections.

Brief History of Ising Model

The Ising model is one of the most broadly studied model in statistical mechanics and provides an example description of a phase transition. This model of ferromagnetism was formulated by Wilhelm Lenz and analysed by his student Ernst Ising in one dimension in 1922 (Brush 1967). Prior to that it was uncertain how to handle phase transitions in ferromagnets theoretically. Ising's (1925) work solved the model in one dimension and established that no phase transition occurs at any non-zero temperature (Wolf 2000; Brush 1967; Kobe 1996). Ising believed the same to be true in other dimensions and stopped

conducting research. This also prompted Heisenberg (1928) to develop his own theory of ferromagnetism with more complex interaction between spins.

Gorsky (1928) attempted to construct a theory by making an hypothesis that the amount of work required to move an atom from an ordered phase to a disordered phase is proportional to the degree of order which already exist. Later, on the basis of Gorsky's theory, Bragg and Williams (1934) investigated the model in effectively infinite dimensions in one of the various approaches to mean field theory (MFT) (discussed in Section 9). Immediately, Bethe (1935) modified the approximation made by Bragg and William by incorporating the short-range ordering between interactions. In the same year, Guggenheim (1935) introduced a new method, called the 'quasi chemical' method, of nearby neighbours interaction in liquids, which was later modified by Rushbrooke (1938).

In 1936, Rudolf Peierls investigated the Ising model and predicted the occurrence of phase transitions in both two and three dimensions (Peierls 1936). However, later his idea was found to be not exact (Griffith 1964). The basic idea is still of interest and since then many mathematicians and scientists have improved and extended the models mentioned above. However, it was not until 1942 that another exact solution to the Ising model was found. It was proposed by the physical chemist Onsager (1944), who found an exact solution for the two dimensional case, in the absence of external magnetic field, using the techniques formulated by Kramers and Wannier (1941).

To this day, no accepted exact solution exists in two dimensions in field, or in three or higher dimensions. Recent claims as to the exact nature of the transition in three dimensions have been made in (Kaupuzs 2001). The mean-field version of the model has, however, been exactly solved and is applicable to infinite-dimensional space (Baxter 2007; McCoy and Wu 1973). The current status of solutions to the Ising model is summarised in Table 4.1. Many mathematical physicists, chemists and biologists have tried to solve the remaining cases of the Ising model, but none yet have succeeded in doing so.

	Dimension				
	d = 1	d = 2	d = 3	d = 4	d ≥ 5
H = 0	✔	✔			Mean Field Theory
H ≠ 0	✔				Mean Field Theory

Table 4.1: Status of exact solution of the Ising Model for various dimensions.

The Ising model remains an important research area and will continue to be so. This is illustrated in the fact that almost one thousand papers are published on this subject each year.

Boundary Conditions

It is required to know about the behaviour of all the boundaries of the system which necessitates the application of boundary conditions. The two possible boundary condition which are discussed here are periodic and free boundary conditions, which are considered for the one and two-dimensional Ising models.

Periodic Boundary Conditions

If periodic boundary conditions are imposed on the one-dimensional system, then there is a link between the Nth site and the first one. Each site is connected with two other links and the system therefore has same number of sites and links. This situation is illustrated in figure 4.5 below. In this situation the system is translationally invariant because all the sites in the system have equivalent properties i.e., the system does not distinguish between the various sites.

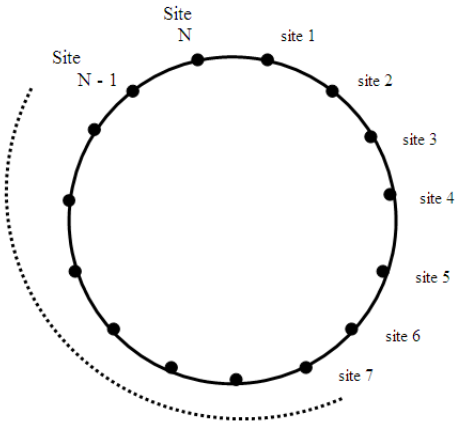

Figure 4.5: One-Dimensional Ising model with periodic boundary conditions

Employing periodic condition for the two-dimensional system, exhibits that every spin in the system is surrouded by four nearby neighbours and interacts with these four nearby spins. This means that the location of the spin on a lattice is not necessary to be known because all the spins exhibits equivalent properties as all the spins are surrounded by the same number of spins. Thus, it can be said that the system is translationally invariant. This is shown in figure 4.6.

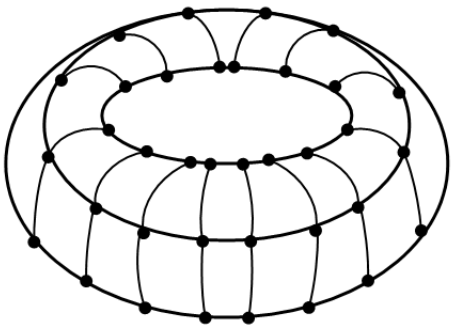

Figure 4.6: Two-Dimensional Ising model with periodic boundary conditions

Free Boundary Conditions

Free boundary conditions are different to those of periodic boundary. In this case, the ends of the system are not joined to each other. As a result, in the case of the one-dimensional system, the first site and the Nth site have only one link whereas the other sites are associated with two links. This scenario is depicted in figure 4.7.

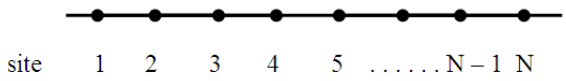

Figure 4.7: One-Dimensional Ising model with free boundary conditions

Since, the ends are not linked with each other, therefore, in case of the two-dimensional system only the middle spins on the lattice has four neighbours and interactions whereas the spins which are located on the outer side of the lattice have either three or two nearest neighbours, as shown in figure 4.8.

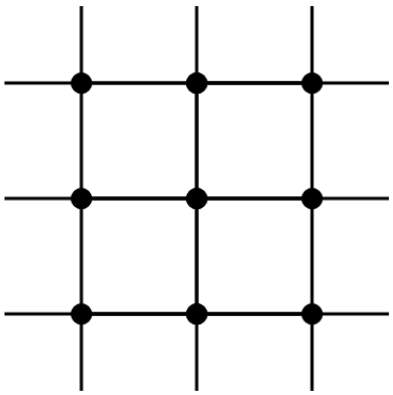

Figure 4.8: Two-dimensional Ising model with free boundary conditions

Thus for such cases the location of the spin is necessary to be known in order to make calculation and assumptions, which makes it more sophisticated and the translational invariance does not hold.

5 Types of Phase Transitions

In section 3, three different examples of phase transitions were discussed. However, there are different types of transitions depending on different types of cases due to the difference in the physical properties. This differing transitions necessitates their classification. The difference between the first and the second order phase transition is discussed. The two classified form of phase transitions are Ehrenfest and the Modern classification.

Ehrenfest Classification

Phase transitions were first classified by P. Ehrenfest (O'Connor and Robertson 2001), on a non-analyticity basis. Under this classification scheme, a first order phase transition is when a discontinuity occurs in the first derivative of the free energy (Gitterman and Halpern 2004). The solid-liquid and the liquid-gas transitions are the examples of first order phase transitions. Since the magnetisation is the first derivative of the free energy with respect to the reduced external field h, figure 5.1 which exhibits a field driven phase transition is also a first order phase transition.

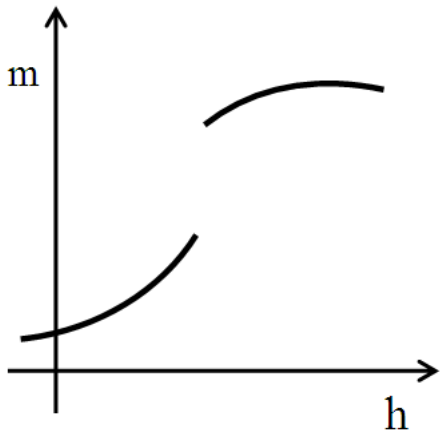

Figure 5.1: An example of field driven phase transition.

In second order phase transitions, the first derivative of the free energy is continuous, however, the discontinuity lies in the second derivative of the free energy. Second order phase transitions include superconductivity and the ferromagnetism transitions. As the first derivative of the specific heat with respect to temperature is continuous and the second derivative is discontinuous, it is said that the specific heat is of second order phase transition. This behaviour of specific heat is illustrated in figure 5.2.

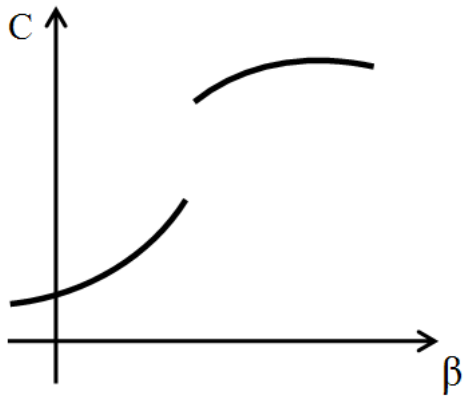

Figure 5.2: The second derivative of the free energy.

Under this classification, besides first and second order transitions, there can be third, fourth and higher-order ones. For nth order phase transitions, the first $n-1$ derivatives of the free energy are continuous and the nth derivative is discontinuous. For the theory of higher order phase transition the reader is referred to Janke, Johnston and Kenna (2006).

Ehrenfest's scheme refers only to discontinuous phase transitions. However, other non-analytic behaviour can occur. For instance, the specific heat diverges near the critical temperature, shown in figure 5.3, and Ehrenfest classification does not take into account such divergent behaviour. This is an addition to Ehrenfest's classification and is usually referred as modern classification of phase transitions.

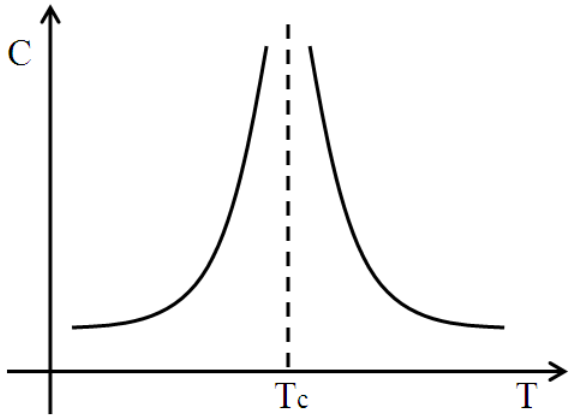

Figure 5.3: Behaviour of specific heat near the critical temperature

Modern Classification

The modern classification in a nutshell, encapsulates first-order and second order phase transitions, which accounts for diverging phase transition. Phase transitions are termed first or higher order irrespective of whether there is an discontinuity or divergence. Second order transitions are also known as continuous phase transitions. The ferromagnetic phase transition is an example of a continuous phase transition (Gitterman and Halpern 2004).

Apart from these two, there also exist infinite order transitions which are continuous transitions that do not break symmetry. These phase transitions include the Kosterlitz-Thouless transition for two-dimensional XY model. Phase transitions of finite order three and higher have not been confirmed experimently, though there is no physical reason why they should not exist. A theoretical study of such transitions is given in Janke, Johnston and Kenna (2006). However, this project is restricted to first and the second order phase transition and the interested reader is referred to Binney *et al.* (2002).

Critical Exponents and Second Order Phase Transitions

Introduced by Verschaffelt (1900), critical exponents describes all the properties of the system when it reaches critical temperature. There are six exponents which defines the behaviour of the thermodynamic functions. Out of these six exponents, the critical exponent β which outlines the behaviour of magnetisation has already been discussed in section 3. Besides β, magnetisation also gives another relationship in terms of δ. This relation is written as

$$m \sim H^{1/\delta} \quad \text{for} \quad T = T_c. \tag{5.1}$$

Another thermodynamic function specific heat, offers another critical exponent which is α. Figure 5.3 exhibit the behaviour of specific heat near the critical temperature and the behaviour satisfies the relationship

$$C \sim |T - T_c|^{-\alpha}, \tag{5.2}$$

This relationship can also be written in terms of the reduced temperature, which is given by

$$C \sim |t|^{-\alpha}. \tag{5.3}$$

The critical behaviour of the magnetic susceptibilty can be characterized as

$$\chi \sim |t|^{-\gamma}. \tag{5.4}$$

All the above thermodynamic variables exhibits the macroscopic properties of the system, however, the microscopic properties provide another perspective about phase transitions. The correlation function is introduced, which describes the relation between any two spins of the system (Parwani 2003). This relation, using the expression (4.9), can be mathematically defined as the difference of the average of the product of two spins and the product of average of two spins, s_i and s_j and is denoted by

$$G(x_i - x_j) = \langle s_i s_j \rangle - \langle s_i \rangle \langle s_j \rangle . \tag{5.5}$$

where the $(x_i - x_j)$ is the separation between the two spins (Ravndal 1976), s_i and s_j. As the distance between the two spin increases i.e., $(x_i - x_j) \to \infty$, the correlation

function approaches towards zero. From the appendix A, the relationship between the susceptibility and the free energy justifies the expression

$$\chi = \frac{1}{N}\left[\frac{1}{Z}\frac{\partial^2 Z}{\partial h^2} - \left(\frac{1}{Z}\frac{\partial Z}{\partial h}\right)^2\right], \tag{5.6}$$

The above expression is then simplified to give

$$\chi = \frac{1}{N}\left[\left\langle M^2\right\rangle - \langle M\rangle^2\right]. \tag{5.7}$$

Since, M is the total magnetisation per configuration, therefore, the above equation can be written as

$$\chi = \frac{1}{N}\sum_i\sum_j \left[\langle s_i s_j\rangle - \langle s_i\rangle \langle s_j\rangle\right]. \tag{5.8}$$

Substituting (5.5) in above result yields

$$\chi = \frac{1}{N}\sum_i\sum_j G(x_i - x_j). \tag{5.9}$$

In the above expression if the term $(x_i - x_j)$ is replaced by x then an extra factor, N, must be introduced in order to modify the expression in terms of only one set. This formulation is given by

$$\chi = \frac{1}{N}N\sum_x G(x), \tag{5.10}$$

$$= \sum_x G(x). \tag{5.11}$$

Thus, this makes both the expressions (5.9) and (5.11) equal. Now, if the distance between the lattice approaches to zero i.e, very small then the summation in the above expression can be replaced by an integral (Ravndal 1976), which gives

$$\chi = \int d^d x G(x). \tag{5.12}$$

This gives an expression for the susceptibility in terms of the correlation function. Further, observing the correlation function experimentally, one can say that the behaviour below and above the critical temperature can be expressed as

$$G(x)|_{T=T_c} \sim x^{-(d-2+\eta)} e^{-x/\xi}. \tag{5.13}$$

This defines the other critical exponent η known as anomalous dimension and ξ known as the correlation length. With the help of the correlation function, the correlation length of the system can be obtained. As shown in figure 5.4, the correlation length is found to be diverging near the critical point.

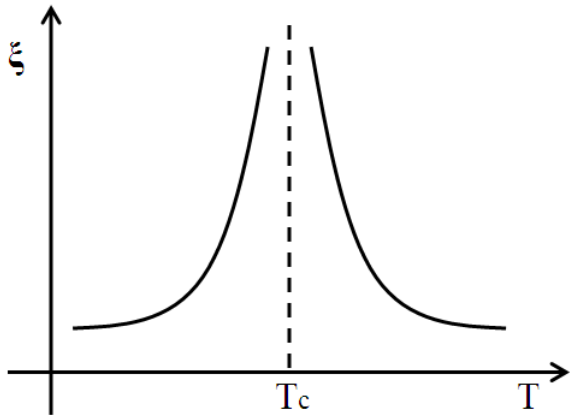

Figure 5.4: Behaviour of correlation length close to the critical temperature

This behaviour can be mathematically written as

$$\xi \sim |t|^{-\nu}. \tag{5.14}$$

where ν is a critical exponent (Ravndal 1976). Having defined the critical behaviour of all thermodynamic functions, the following table summaries all the critical exponents:

Thermodynamic Function	Symbol	Definition	Behaviour
Magnetisation	m	$\frac{\partial f}{\partial h}$	$m \sim \lvert t\rvert^{\beta}$
Magnetisation	m	$\frac{\partial f}{\partial h}$	$m \sim \lvert H\rvert^{1/\delta}$
Susceptibility	χ	$\frac{\partial^2 f}{\partial h^2}$	$\chi \sim \lvert t\rvert^{-\gamma}$
Specific Heat	C	$\frac{\partial^2 f}{\partial \beta^2}$	$C \sim \lvert t\rvert^{-\alpha}$
Correlation Function	$G(x)$	$\langle s_i s_j\rangle - \langle s_i\rangle \langle s_j\rangle$	$G(x) \sim x^{-(d-2+\eta)} e^{-x/\xi}$
Correlation Length	ξ		$\xi \sim \lvert t\rvert^{-\nu}$

Table 5.1: Critical Behaviour of Thermodynamic Functions

6 Other Statistical Mechanical Models

There are several other models, apart from the Ising model, in statistical mechanics which play important roles in the theory of phase transitions. In order to contrast them with the Ising model, some of these are outlined briefly below.

The Potts Model

The Potts model is an extension of the Ising model. While the Ising model consists of spins which can take two different values, the Potts model spins can have q different values (Potts 1952). The interaction energy between the nearby spins is non-zero, if they have the same value and the interaction energy is zero if the values are different. Thus, the Potts model is same as the Ising model when $q = 2$ (Wu 1982). In two dimensions when $q \leq 4$ there occurs a temperature-driven transition which is continuous and this continuous transition is identical to the Ising transition when $q = 2$. The transition is of first order if $q > 4$ and when $q < 4$ the transition is either of first or the second order in various dimensions. Table 6.1 below exhibits different transitions when $q < 4$.

Dimensions → / q values ↓	d = 1	d = 2	d = 3	d = 4	d ≥ 5
q = 2 (Ising)	No Phase Transition	2nd order Phase Transition	2nd order Phase Transition	2nd order Phase Transition	2nd order Phase Transition
q = 3		2nd order Phase Transition	1st order Phase Transition	1st order Phase Transition	1st order Phase Transition
q = 4		2nd order Phase Transition	1st order Phase Transition		
q = 5		1st order Phase Transition	1st order Phase Transition		

Table 6.1: Different transitions in various dimensions

The XY Model

The XY model is an arrangement of spins on a d-dimensional lattice where the spins lie in a plane and have fixed length. In this case, the spins in the system are described by two component vector (Binney *et al.* 2002). According to the Mermin - Wagner theorem (1966), there occurs no long-range order in such a system in two dimensions. However, Kosterlitz and Thouless (1973) showed the occurrence of a phase transition for this model causes by '*topological excitations of vortex-antivortex pairs*'.

The Heisenberg Model

In case of the Heisenberg model, the spins on each lattice site, like XY model, also have a freedom to move in any direction. This model consists of spins in D dimensions and the XY model can be obtained when $D = 2$.

General O(n) models

The general O(n) models consists of spins placed on d-dimensional lattice. The spins at each site has n possible directions to exist in the system and the XY and general Heisenberg model are obtained when $n = 2$ and $n = 3$.

On the basis of the assumptions made within the models, as discussed above, all the critical exponents can be obtained. The values for all the critical exponents for these models and 2-d and 3-d Ising model have been listed in table 6.2, however, for the derivations for these the reader is referred to Plischke and Bergersen (2006), Domb and Lebowitz (2001) and Binney *et al.* (2002).

Statistical Models	α	β	γ	δ	ν	η
2-d Ising	0 (log)	$\frac{1}{8}$	$\frac{7}{4}$	15	1	$\frac{1}{4}$
3-d Ising	$\approx \frac{1}{8}$	$\approx \frac{5}{16}$	$\approx \frac{5}{4}$	≈ 5	$\approx \frac{5}{8}$	≈ 0
2-d Potts Model q = 4	$\frac{2}{3}$	$\frac{1}{12}$	$\frac{7}{6}$	15	$\frac{2}{3}$	$\frac{1}{2}$
XY Model d = 3	0.01	0.34	1.30	4.8	0.66	0.04
Heisenberg Model d = 3	- 0.12	0.36	1.39	4.8	0.71	0.04

Table 6.2: Values of Critical Exponents of Various Statistical Mechanical Models

Universality

When two systems of different specifications have the same critical exponents, it is known as Universality. This states that the critical exponents of any system are not dependent on the microscopic details of that system, instead they depend on the dimensionality of the system and the spins and also on the interaction range. Therefore, large systems can be simplified using models with the same dimensionality and interaction range.

7 Scaling Relations

In the early sixties four relationships between the six critical exponents were developed (see e.g., Binney *et al.* 2002). The original relationships were three inequalities and one equality, namely

$$\nu d \geq 2 - \alpha, \tag{7.1}$$

$$2\beta + \gamma \geq 2 - \alpha, \tag{7.2}$$

$$\beta(\delta - 1) \leq \gamma, \tag{7.3}$$

$$\gamma = \nu(2 - \eta). \tag{7.4}$$

In 1965, Widom proved the first and the third inequalities to be equalities (Binney *et al.* 2002) and Essam and Fisher in 1963 proved the second relation to be an equality. Here, in this section these four scaling relations are developed. The first relation is known as Josephson's Law (Widom 1965, Kadanoff 1966 and Josephson 1967) and using the hyper-scaling hypothesis its derivation can be obtained. In this case the dimensionality plays an important role and the relation turns out to be valid only for dimensions less than or equal to four. Alternatively, this can also be derived from the Kadanoff block-spin construction (see e.g., Ravndal 1976). Next, the other two scaling relations, known as Rushbrooke's Law (Essam and Fisher 1963, Rushbrooke 1963)and Griffith's Law (Widom 1964 and Griffiths 1965), can be obtained using the Widom scaling hypothesis where the free energy is a homogeneous function (see e.g., Ravndal 1976). The remaining Fisher equality (Fisher 1964) is also presented.

Hyperscaling Hypothesis

In order to derive the first scaling relation, the free energy is assumed to behave as the inverse of the correlation volume such that

$$f \sim \xi^{-d}. \tag{7.5}$$

The above assumption is known as hyperscaling hypothesis. This expression can be modified using the expression for correlation length in (5.14), which gives

$$f \sim |t|^{\nu d}. \tag{7.6}$$

Since the specific heat is the second derivative of the free energy, differentiating with respect to t yields

$$C \propto |t|^{\nu d-2}. \tag{7.7}$$

Comparing this with the behavior of specific heat in (5.3) results in the equality

$$\nu d = 2 - \alpha. \tag{7.8}$$

This is known as Josephson's Law and was formulated in 1960's.

Next, considering the behaviour of correlation function as in (5.13) and substituting the value for $G(x)$ in (5.12) gives another scaling relation.

$$\chi \sim \int_0^{\xi} d^d x x^{-(d-2+\eta)} e^{-x/\xi}, \tag{7.9}$$

having introduced ξ as the upper integral limit, following the original work of Fisher (1964). Now converting the above expression to polar coordinates yields

$$\chi \sim \int_0^{\xi} r^{d-1} dr r^{-(d-2+\eta)} e^{-r/\xi}, \tag{7.10}$$

having integrated over the angular coordinates. This integral gives

$$\begin{aligned} \chi &\sim r^{2-\eta} e^{-r/\xi}|_0^{\xi}, \\ &\sim \xi^{2-\eta}. \end{aligned} \tag{7.11}$$

Substituting the expression for ξ from (5.14) in the above result yields

$$\chi \sim |t|^{-\nu(2-\eta)}. \tag{7.12}$$

Comparing this with the behaviour of susceptibility in (5.4) results another scaling relation:

$$\gamma = \nu(2 - \eta). \tag{7.13}$$

This equality is known as Fisher's Law.

Widom Scaling Hypothesis

Using an assumption of homogeneous functions the remaining two relations can be obtained. Suppose $F(x)$ is a homogeneous function of one variable, which means that if x is multiplied with an arbitrary factor λ, the value of the function $F(x)$ is then rescaled by a function of λ, i.e.,

$$F(\lambda x) = g(\lambda)F(x). \tag{7.14}$$

Now rescaling again, by a factor μ gives

$$\begin{aligned} F(\lambda\mu x) &= F(\lambda(\mu x)), \\ &= g(\lambda)F(\mu x), \\ &= g(\lambda)g(\mu)F(x). \end{aligned} \tag{7.15}$$

Applying the property (7.14) to the left hand side of (7.15) gives

$$F(\lambda\mu x) = g(\lambda\mu)F(x). \tag{7.16}$$

Thus, comparing the above expressions gives

$$g(\lambda\mu) = g(\lambda)g(\mu). \tag{7.17}$$

So differentiating this with respect to μ yields

$$\lambda g'(\lambda\mu) = g(\lambda)g'(\mu). \tag{7.18}$$

Now, choosing $\mu = 1$ and $g'(1) = p$, the above differentiation equals

$$\lambda g'(\lambda) = g(\lambda)p. \tag{7.19}$$

or

$$\frac{g'(\lambda)}{g(\lambda)} = \frac{p}{\lambda}. \tag{7.20}$$

Since the differentiation of $\ln g(\lambda)$ with respect to λ is same as the right hand side of the above expression, therefore, this can be alternatively written as

$$\frac{d}{d\lambda}\ln g(\lambda) = \frac{p}{\lambda}, \tag{7.21}$$

Integrating this results in

$$\ln g(\lambda) = p \ln \lambda + c, \tag{7.22}$$

or alternatively

$$g(\lambda) = e^c e^{p \ln \lambda}, \tag{7.23}$$

$$\sim \lambda^p. \tag{7.24}$$

Therefore a homogeneous function for one variable involves a power like behaviour i.e.,

$$F(\lambda x) \sim \lambda^p F(x). \tag{7.25}$$

Rewriting λ as $\lambda'^{1/p}$ in above gives

$$F(\lambda'^{1/p} x) = \lambda' F(x), \tag{7.26}$$

Let $a = 1/p$ and rename λ' as λ:

$$F(\lambda^a x) = \lambda F(x). \tag{7.27}$$

Similarly, this also holds true for multi-variable functions i.e.,

$$F(\lambda^a x, \lambda^b y) = \lambda F(x, y). \tag{7.28}$$

Now, recalling the expression for the free energy as in (4.15) and writing in terms of reduced external field and reduced temperature, yields

$$f(t, h) = \frac{-kT}{N} \ln Z(t, h). \tag{7.29}$$

Now, making an assumption that close to the critical point the free energy consists of regular, f_R and a singular, f_S part, which is

$$f(t, h)|_{T \to T_c} = f_R(t, h)|_{T \to T_c} + f_S(t, h)|_{T \to T_c}. \tag{7.30}$$

Further, again assuming that the singular function of the free energy to be a homogeneous function:

$$f(\lambda^a t, \lambda^b h) = \lambda f(t, h), \tag{7.31}$$

The above hypothesis is called Widom Scaling for the free energy. Since the generalised homogeneity was expressed in terms of parameters a and b, the critical exponents are evaluated in terms of the same parameters. From (4.16), the magnetisation is given to be a first derivative of the free energy with respect to h, therefore differentiating the above expression yields

$$\lambda^b m(\lambda^a t, \lambda^b h) = \lambda m(t, h). \tag{7.32}$$

If the external field approaches zero then this becomes

$$m(t, 0) = \lambda^{b-1} m(\lambda^a t, 0). \tag{7.33}$$

Choose $\lambda = (-t)^{-1/a}$ as t is negative. Substituting this in above expression gives

$$m(t, 0) = (-t)^{(1-b)/a} m(-1, 0). \tag{7.34}$$

The critical exponent β can now be identified by comparing the above equation with the behaviour of β. Doing this gives β to be

$$\beta = \frac{1-b}{a}. \tag{7.35}$$

Similarly, the critical exponent δ can also be evaluated. So letting t = 0 in (7.32) gives

$$\lambda^b m(0, \lambda^b h) = \lambda m(0, h), \tag{7.36}$$

and if λ is replaced by $h^{-1/b}$ then this simplifies to

$$\begin{aligned} m(0, h) &= \lambda^{b-1} m(0, \lambda^b h), \\ &= h^{\frac{1-b}{b}} m(0, 1). \end{aligned} \tag{7.37}$$

As before, comparing this with the defination of δ gives

$$\delta = \frac{b}{1-b}. \tag{7.38}$$

Next in order to find the exponent γ, consider the behaviour of the susceptibility which is the second derivative of the free energy with respect to h. Following this the second derivative of the free energy from (7.31) is

$$\lambda^{2b} \chi(\lambda^a t, \lambda^b h) = \lambda \chi(t, h). \tag{7.39}$$

In the absence of external field and above the critical temperature, this becomes

$$\lambda^{2b}\chi(\lambda^a t, 0) = \lambda\chi(t, 0). \tag{7.40}$$

Choosing $\lambda = (t)^{-1/a}$ and replacing this in above yields

$$\chi(t, 0) = t^{(1-2b)/a}\chi(1, 0). \tag{7.41}$$

Comparing this with the behaviour of the susceptibility then,

$$\gamma = \frac{2b - 1}{a}. \tag{7.42}$$

Below the critical temperature the value for the susceptibility exponent is same as the γ. Now rearranging the expressions for β and δ to give a and b:

$$b = \frac{\delta}{1 + \delta}, \tag{7.43}$$

and

$$\begin{aligned} a &= \frac{1 - b}{\beta}, \\ &= \frac{1 - \frac{\delta}{1+\delta}}{\beta}, \\ &= \frac{1}{\beta(1 + \delta)}. \end{aligned} \tag{7.44}$$

Substituting these results into (7.42) gives

$$\begin{aligned} \gamma &= \frac{2(\frac{\delta}{1+\delta}) - 1}{\frac{1}{\beta+\beta\delta}}, \\ &= \frac{\beta(1 + \delta)(\delta - 1)}{(1 + \delta)}, \\ \gamma &= \beta(\delta - 1). \end{aligned} \tag{7.45}$$

This simplification gives the third scaling relation which is known as Griffith's Law and was formulated 1965.

Next to find the last scaling relation consider the specific heat, which is the second derivative of the free energy with respect to t. Differentiating (7.31) gives

$$\lambda^{2a}C(\lambda^a t, \lambda^b h) = \lambda C(t, h). \tag{7.46}$$

In the absence of external field this results in

$$\lambda^{2a} C(\lambda^a t, 0) = \lambda C(t, 0). \tag{7.47}$$

and choosing $\lambda = (t)^{-1/a}$ simplifies to

$$C(t, 0) = t^{(1-2a)/a} C(1, 0). \tag{7.48}$$

The critical exponent α is then found by comparing the above expression with the behaviour of the specific heat:

$$\alpha = \frac{2a - 1}{a}. \tag{7.49}$$

Substituting the value of a in this yields

$$\begin{aligned} \alpha &= \frac{\frac{2}{\beta+\beta\delta} - 1}{\frac{1}{\beta+\beta\delta}}, \\ &= 2 - \beta(\delta + 1). \end{aligned} \tag{7.50}$$

The above expression is the last scaling relation known as Rushbrooke's Law and was found in 1963. Thus, all the scaling inequalities have been proved as equality and these equalities has been illustrated below.

Scaling Relations	
Josephson's Law	$vd = 2 - \alpha$
Rushbrooke's Law	$2\beta + \gamma = 2 - \alpha$
Griffith's Law	$\beta\,(\delta - 1) = \gamma$
Fisher's Law	$\gamma = \nu(2 - \mu)$

Table 7.1: Four scaling relations

Josephson's Law fails above $d = 4$. This is discussed in chapter 9.

8 One-Dimensional Ising Model

Guided by W.Lenz, E. Ising solved the model in one dimension showing that no phase transition occurs at any non-zero temperature (Ising 1925). Deriving the exact results for the Ising model in one dimension is one of the objectives of this project. The technique which has been considered throughout the calculations for one dimension in this section is the transfer matrix technique, introduced by Kramers and Wannier (1941). The concept of this technique is to first write the partition function in terms of a matrix, known as the transfer matrix and then calculate its eigenvalues. With the help of these eigenvalues it is then simple to derive all the thermodynamic functions. Following the method (i) the critical exponents are derived, (ii) the scaling relations are examined and (iii) it is shown that no phase transition occurs at $T \neq 0$.

As discussed in section 4, if periodic boundary conditions are imposed on system in one dimension, then there is a link between the N^{th} site and the first one, i.e., the system has same number of sites and links. This scenario is depicted in figure 4.5. In this situation the system is translationally invariant because all the sites in the system have equivalent properties. Now the magnetisation, with respect to temperature and external field, from (4.8) can be expressed as an average of magnetic spin per site which is

$$m(H,T) = \frac{1}{N}\left\langle s_1 + s_2 + \cdots s_N \right\rangle, \tag{8.1}$$

Since the system is translationally invariant, the average magnetisation of every spin will be the similar to the neighbouring spins. Thus the magnetisation can be written as

$$m(T,H) = \langle s_1 \rangle = \langle s_2 \rangle = ... = \langle s_N \rangle, \tag{8.2}$$

or this can also be rewritten, in terms of s_i which is assumed to be any site of the system, as

$$m(T,H) = \langle s_i \rangle. \tag{8.3}$$

Substituting the expression for the energy and total magnetisation in (4.14) gives

$$Z_N = \sum_{\{s_i\}} \exp\left(K \sum_{<i,j>} s_i s_j + h \sum_i s_i \right). \tag{8.4}$$

where $K = J/kT$, $h = H/kT$ and the summation is over all configurations which the system can be in. Now, the first exponent is

$$\sum_{<i,j>} s_i s_j = s_1 s_2 + s_2 s_3 + ... + s_{N-1} s_N + s_N s_1 = \sum_{i=1}^{N} s_i s_{i+1}. \tag{8.5}$$

As a result, the partition function can now be written as

$$Z_N = \sum_{\{s_i\}} \exp\left(K \sum_{i=1}^{N} s_i s_{i+1} + h \sum_i s_i \right), \tag{8.6}$$

Now clearly $\sum_i s_i = \sum_i s_{i+1}$, so

$$\sum_i s_i = \frac{1}{2} \sum_i (s_i + s_{i+1}). \tag{8.7}$$

Substituting this in the previous expression for the partition function, one has

$$Z_N = \sum_{\{s_i\}} \exp\left(K \sum_{i=1}^{N} s_i s_{i+1} + \frac{h}{2} \sum_i (s_i + s_{i+1}) \right). \tag{8.8}$$

Keeping in mind the two nearby spins the exponential in (8.8) can be factored giving

$$\begin{aligned} Z_N &= \sum_{\{s_i\}} e^{[K s_1 s_2 + \frac{h}{2}(s_1 + s_2) + K s_2 s_3 + \frac{h}{2}(s_2 + s_3) + \cdots + K s_N s_1 + \frac{h}{2}(s_N + s_1)]}, \\ &= \sum_{\{s_i\}} e^{K s_1 s_2 + \frac{h}{2}(s_1 + s_2)} . e^{K s_2 s_3 + \frac{h}{2}(s_2 + s_3)} \cdots e^{K s_N s_1 + \frac{h}{2}(s_N + s_1)}. \end{aligned} \tag{8.9}$$

With s_i and s_j any two neighbouring sites of the system, write

$$V(s_i, s_j) = e^{K s_i s_j + \frac{h}{2}(s_i + s_j)}. \tag{8.10}$$

The partition function can now be expressed as

$$Z_N = \sum_{\{s_i\}} V(s_1, s_2) \cdot V(s_2, s_3) \cdots V(s_{N-1}, s_N) V(s_N, s_1). \tag{8.11}$$

Since the s_i, s_j in (8.10) can only take value from the set $\{\pm 1\}$, there are only four possible arrangements for a pair of spins i.e, both positive, both negative and two sets of positive and negative. As a result, using these arrangements $V(s_i, s_j)$ can be expressed as an element of a 2×2 matrix:

$$\begin{aligned} V &= \begin{pmatrix} V(1,1) & V(1,-1) \\ V(-1,1) & V(-1,-1) \end{pmatrix}, \\ &= \begin{pmatrix} e^{K+h} & e^{-K} \\ e^{-K} & e^{K-h} \end{pmatrix}. \end{aligned} \tag{8.12}$$

Now using the multiplication property of matrices on the $s_2, s_3, \cdots, s_N$ and the summation over s_1 is expressed as

$$Z_N = \sum_{\{s_i\}} V^N = \mathrm{Tr} V^N. \tag{8.13}$$

Now, let $\vec{x}$ and $\vec{y}$ be the two eigenvectors of V

$$\vec{x} = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \quad \text{and} \quad \vec{y} = \begin{pmatrix} y_1 \\ y_2 \end{pmatrix}$$

and λ_1 and λ_2 be the corresponding eigenvalues, such that

$$V\vec{x} = \lambda_1 \vec{x}, \quad \text{and} \quad V\vec{y} = \lambda_2 \vec{y}. \tag{8.14}$$

Considering another a 2×2 matrix R such that

$$R = \begin{pmatrix} x_1 & y_1 \\ x_2 & y_2 \end{pmatrix}. \tag{8.15}$$

In order to satisfy the two expressions in (8.14), first consider the multiplication of matrix V and R:

$$\begin{aligned} VR &= \begin{pmatrix} V_{11} & V_{12} \\ V_{21} & V_{22} \end{pmatrix} \begin{pmatrix} x_1 & y_1 \\ x_2 & y_2 \end{pmatrix}, \\ &= \begin{pmatrix} V_{11}x_1 + V_{12}x_2 & V_{11}y_1 + V_{12}y_2 \\ V_{21}x_1 + V_{22}x_2 & V_{21}y_1 + V_{22}y_2 \end{pmatrix}. \end{aligned} \tag{8.16}$$

and next multiply the matrix R with an eigenvalue matrix giving

$$\begin{aligned} R \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} &= \begin{pmatrix} x_1 & y_1 \\ x_2 & y_2 \end{pmatrix} \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}, \\ &= \begin{pmatrix} x_1\lambda_1 & y_1\lambda_2 \\ x_2\lambda_1 & y_2\lambda_2 \end{pmatrix}. \end{aligned} \tag{8.17}$$

Comparing the first column of the above multiplications yields

$$V_{11}x_1 + V_{12}x_2 = \lambda_1 x_1,$$

$$V_{21}x_1 + V_{22}x_2 = \lambda_1 x_2.$$

which implies

$$V\vec{x} = \lambda_1 \vec{x}.$$

Similarly, comparing the second column satisfies both the expressions in (8.14). This results that the above multiplications are equal and can be written as

$$VR = R \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}. \tag{8.18}$$

Next multiplying both sides of (8.18) with R^{-1} gives

$$V = R \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} R^{-1}, \tag{8.19}$$

The power of V in (8.13) now reads

$$\begin{aligned} V^N &= R \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} R^{-1} \cdots R \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} R^{-1}, \\ &= R \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}^N R^{-1}. \end{aligned} \tag{8.20}$$

Using the cyclic properties of trace, R in above cancels out, leaving only the trace of two-by-two matrix. Thus, the partition function becomes

$$Z_N = \mathrm{Tr} \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}^N. \tag{8.21}$$

Since the trace of a matrix is equal to the sum of the diagonal terms, therefore, the above equation equivalently can be written as

$$Z_N = \lambda_1^N + \lambda_2^N. \tag{8.22}$$

To obtain the values of both the eigenvalues, one writes the characteristic equation of V as

$$\det(V - \lambda I) = 0. \tag{8.23}$$

In detail,

$$\det \begin{pmatrix} e^{K+h} - \lambda & e^{-K} \\ e^{-K} & e^{K-h} - \lambda \end{pmatrix} = 0,$$

giving

$$(e^{K+h} - \lambda)(e^{K-h} - \lambda) - e^{-2K} = 0.$$

Expanding gives a quadratic equation namely

$$\lambda^2 - \lambda e^K (e^h + e^{-h}) + e^{2K} - e^{-2K} = 0. \tag{8.24}$$

The solution is

$$\lambda = \frac{e^K(e^h + e^{-h}) \pm \sqrt{e^{2K}(e^h + e^{-h})^2 - 4(e^{2K} - e^{-2K})}}{2}.$$

Now using the hyperbolic functions and trigonometric identity of sinh, this becomes

$$\begin{aligned} \lambda &= e^K \cosh h \pm \sqrt{e^{2K}\cosh^2 h - e^{2K} + e^{-2K}}, \\ &= e^K \cosh h \pm \sqrt{e^{2K}\sinh^2 h + e^{-2K}}. \end{aligned} \tag{8.25}$$

Free Energy

Next consider one of the eigenvalues, let say λ_1 to be the larger of the two, and write (8.22) as

$$Z_N = \lambda_1^N \left(1 + \frac{\lambda_2^N}{\lambda_1^N}\right).$$

Taking logarithm on both sides gives

$$\ln Z_N = \ln \left[\lambda_1^N \left(1 + \left(\frac{\lambda_2}{\lambda_1}\right)^N\right)\right],$$

which is equivalent to

$$N^{-1} \ln Z_N = \ln \lambda_1 + N^{-1} \ln \left[1 + \left(\frac{\lambda_2}{\lambda_1}\right)^N\right]. \tag{8.26}$$

As N tends to infinity, therefore, second logarithm term on the right hand side of the above equation approaches zero. Thus, substituting this result in the expression for free energy, as earlier discussed in section 4, yields

$$\begin{aligned} f(H,T) &= -kT \lim_{N\to\infty} N^{-1} \ln Z_N, \\ &= -kT \ln \lambda_1, \end{aligned}$$

Replacing λ_1 by (8.25) in the above expression results

$$f(H,T) = -kT\ln[e^K \cosh h + \sqrt{e^{2K}\sinh^2 h + e^{-2K}}]. \tag{8.27}$$

The above equation is an expression for the free energy which has been defined in terms of H and T.

Magnetisation

The magnetisation can be expressed as the negative first derivative of free energy with respect to external field H. This can be expanded and written as

$$m = -\frac{\partial f}{\partial H} = -\frac{\partial f}{\partial h}\frac{\partial h}{\partial H}. \tag{8.28}$$

In order to obtain an expression for the magnetisation for one-dimensional model differentiate the free energy (8.27) with respect to h and the reduced external field (4.13) with respect to H. As a result, the free energy now given as

$$\begin{aligned}
\frac{\partial f}{\partial h} &= \frac{-kT[e^K \sinh h + e^{2K}\sinh h \cosh h(e^{2K}\sinh^2 h + e^{-2K})^{-1/2}]}{[e^K \cosh h + (e^{2K}\sinh^2 h + e^{-2K})^{1/2}]}, \\
&= \frac{-kTe^K \sinh h[(e^{2K}\sinh^2 h + e^{-2K})^{1/2} + e^K \cosh h]}{[e^{2K}\sinh^2 h + e^{-2K}]^{1/2}[e^K \cosh h + (e^{2K}\sinh^2 h + e^{-2K})^{1/2}]}, \\
&= \frac{-kTe^K \sinh h}{[e^{2K}\sinh^2 h + e^{-2K}]^{1/2}}.
\end{aligned} \tag{8.29}$$

and the reduced external field now written as

$$\frac{\partial h}{\partial H} = \beta. \tag{8.30}$$

Substituting the last two results in (8.28) gives

$$m(H,T) = \frac{e^K \sinh h}{[e^{2K}\sinh^2 h + e^{-2K}]^{1/2}}. \tag{8.31}$$

The above equation is an expression for the magnetisation defined in terms of temperature and the external magnetic field.

Correlations

Next the solution for the correlation length ξ will be discussed. From (4.11) the probability that the system is in a state 's_i' is

$$Z^{-1}e^{-E(s_i)/kT} = Z_N^{-1}V(s_1, s_2)V(s_2, s_3)V(s_3, s_4)\dots V(s_N, s_1). \tag{8.32}$$

In particular, the average of the product of any two spins in the system, for instance $s_1 s_3$, is

$$\langle s_1 s_3\rangle = Z_N^{-1}\sum_{s_i} s_1 V(s_1, s_2)V(s_2, s_3)s_3 V(s_3, s_4)\dots V(s_N, s_1). \tag{8.33}$$

Using the previous notations, the above expression can also be expressed in the form of a matrix. Now defining another two by two diagonal matrix A in terms of s_i and s_j such that it is equal to $s_i\delta(s_i, s_j)$ where $\delta(s_i, s_j)$ is

$$\begin{cases} 1 & s_i = s_j \\ 0 & s_i \neq s_j \end{cases}.$$

Therefore, the matrix A can be written as

$$A = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{8.34}$$

Now taking trace of expression (8.33) and using (8.34), the average of spins becomes

$$\langle s_1 s_3\rangle = Z_N^{-1}TrAVVAV\cdots V = Z_N^{-1}TrAV^2AV^{N-2}. \tag{8.35}$$

Similarly, the average value of $s_i s_j$ and the individual spin s_i would be

$$\langle s_i s_j\rangle = Z_N^{-1}TrAV^{j-i}AV^{N+i-j}, \tag{8.36}$$

and

$$\langle s_i\rangle = Z_N^{-1}TrAV^N. \tag{8.37}$$

The average value of $s_i s_j$ is dependent on i and j and the s_i is independent of i. Thus it is clear that the two equations exhibits the translational invariance behaviour.

Next substituting the value of V in the first expression of (8.14) yields

$$\begin{pmatrix} e^{K+h} & e^{-K} \\ e^{-K} & e^{K-h} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \lambda_1 \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}, \tag{8.38}$$

Multiplying the matrices on left hand side gives

$$e^{K+h}x_1 + e^{-K}x_2 = \lambda_1 x_1, \tag{8.39}$$

Rearranging the equation in order to form a fraction of x_1 and x_2 and substituting the value for λ_1 gives

$$\frac{x_2}{x_1} = e^K \left[e^K \cosh h + \sqrt{e^{2K} \sinh^2 h + e^{-2K}} - e^{K+h} \right], \tag{8.40}$$

Using the hyperbolic function for sinh and cosh, the above fraction becomes

$$\frac{x_2}{x_1} = \sqrt{e^{4K} \sinh^2 h + 1} - e^{2K} \sinh h. \tag{8.41}$$

Defining any number ϕ, which lies between 0 and $\pi/2$, by

$$\cot 2\phi = e^{2K} \sinh h, \tag{8.42}$$

and substituting this into (8.41) yields

$$\begin{aligned} \frac{x_2}{x_1} &= (\cot^2 2\phi + 1)^{1/2} - \cot 2\phi, \\ &= \operatorname{cosec} 2\phi - \cot 2\phi, \end{aligned} \tag{8.43}$$

Using the trigonometric identities results in

$$\begin{aligned} \frac{x_2}{x_1} &= \frac{1}{\sin 2\phi} - \frac{\cos 2\phi}{\sin 2\phi}, \\ &= \frac{1 - (2\cos^2 \phi - 1)}{2 \sin \phi \cos \phi}, \end{aligned} \tag{8.44}$$

which can be equivalently written as

$$\frac{x_2}{x_1} = \frac{\sin \phi}{\cos \phi}. \tag{8.45}$$

Therefore, the value of the eigenvectors x_1 and x_2 is choosen to be $\cos\phi$ and $\sin\phi$. Similarly, the other eigenvectors can be obtained and following the procedure yields $\vec{y}$ of (8.14) to be $-\sin\phi$ and $\cos\phi$. Arranging the eigenvectors forms an orthogonal matrix R as

$$R = \begin{pmatrix} \cos\phi & -\sin\phi \\ \sin\phi & \cos\phi \end{pmatrix}. \tag{8.46}$$

Using matrix inverse formula, the inverse of square matrix R is then given by

$$R^{-1} = \frac{1}{\cos^2\phi + \sin^2\phi} \begin{pmatrix} \cos\phi & \sin\phi \\ -\sin\phi & \cos\phi \end{pmatrix}. \tag{8.47}$$

The matrix V and A in expression (8.36) and (8.37) remains to be the same even if they are replaced by (8.19). Therefore, using the inverse of R, the matrix V can be written as

$$R^{-1}VR = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}, \tag{8.48}$$

and A is written as

$$\begin{aligned} R^{-1}AR &= \begin{pmatrix} \cos\phi & \sin\phi \\ -\sin\phi & \cos\phi \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \cos\phi & -\sin\phi \\ \sin\phi & \cos\phi \end{pmatrix}, \\ &= \begin{pmatrix} \cos^2\phi - \sin^2\phi & -2\sin\phi\cos\phi \\ -2\sin\phi\cos\phi & \sin^2\phi - \cos^2\phi \end{pmatrix}, \end{aligned} \tag{8.49}$$

Using the trigonometric identities in the above matrix gives a more simplified version, which is

$$R^{-1}AR = \begin{pmatrix} \cos 2\phi & -\sin 2\phi \\ -\sin 2\phi & -\cos 2\phi \end{pmatrix}, \tag{8.50}$$

Taking the limit $N \to \infty$ and keeping $j - i$ fixed, substitute the above expressions into (8.36) and (8.37). Using the matrix multiplication property, first multiplying the matrices, then taking their trace and finally substituting the expression for the partition function gives an expression for the average value of $s_i s_j$:

$$\begin{aligned} \langle s_i s_j \rangle &= Z_N^{-1} Tr R^{-1}AR(R^{-1}VR)^{j-i}R^{-1}AR(R^{-1}VR)^{N+i-j}, \\ &= Z_N^{-1}\left[\lambda_1^N \cos^2 2\phi + \lambda_1^{N+i-j}\lambda_2^{j-i}\sin^2 2\phi + \lambda_1^{j-i}\lambda_2^{N+i-j}\sin^2 2\phi + \lambda_2^N \cos^2 2\phi\right], \end{aligned}$$

$$
\begin{aligned}
&= \frac{[\lambda_1^N + \lambda_2^N]\left[\cos^2 2\phi + \sin^2 2\phi(\lambda_2/\lambda_1)^{j-i}\right]}{\lambda_1^N + \lambda_2^N}, \\
&= \cos^2 2\phi + \sin^2 2\phi \left(\frac{\lambda_2}{\lambda_1}\right)^{j-i}. \qquad (8.51)
\end{aligned}
$$

Similarly, the average value of s_i can be obtained. This is given by

$$
\begin{aligned}
\langle s_i \rangle &= Z_N^{-1} \mathrm{Tr} R^{-1} A R (R^{-1} V R)^N, \\
&= \frac{\cos 2\phi(\lambda_1^N - \lambda_2^N)}{\lambda_1^N + \lambda_2^N}, \\
&= \frac{\cos 2\phi(1 - (\lambda_2/\lambda_1)^N)}{(1 + (\lambda_2/\lambda_1)^N)}, \qquad (8.52)
\end{aligned}
$$

Again using the fact that ${\lambda_2/\lambda_1}^N$ approaches zero in the infinite volume limit,

$$\langle s_i \rangle = \cos 2\phi. \qquad (8.53)$$

This expression is an alternative equation for magnetisation which is equivalent to (8.31). Next, the correlation function 'g_{ij}' can be found by substituting the values for the averages from (8.51) and (8.53) in (5.5) yields

$$
\begin{aligned}
g_{ij} &= \langle s_i s_j \rangle - \langle s_i \rangle \langle s_j \rangle, \\
&= \sin^2 2\phi \left(\frac{\lambda_2}{\lambda_1}\right)^{j-i}. \qquad (8.54)
\end{aligned}
$$

Finally using the above expression the correlation length ξ can be found. Since the eigenvector λ_1 is greater than λ_2, therefore it can be noticed that the correlation function tends exponentially to zero. As a result, the exponential in the above expression yields

$$
\begin{aligned}
g_{ij} &= \sin^2 2\phi e^{\ln(\lambda_2/\lambda_1)^{j-i}}, \\
&= \sin^2 2\phi e^{|j-i| \ln(\lambda_2/\lambda_1)},
\end{aligned}
$$

From (5.13) letting $(j - i)$ be r then the correlation scale as

$$g(r) \sim e^{-r \ln(\lambda_1/\lambda_2)}. \qquad (8.55)$$

Therefore, comparing with (5.13) gives an expression for correlation length ξ. I.e.,

$$\xi = \left[\ln\left(\frac{\lambda_1}{\lambda_2}\right)\right]^{-1}. \qquad (8.56)$$

Critical Behaviour near $T = 0$

The correlation length diverges when

$$\frac{\lambda_1}{\lambda_2} = 1. \tag{8.57}$$

Substituting the value of λ_1 and λ_2 and setting $h = 0$, the above expression becomes

$$e^K + e^{-K} = e^K - e^{-K}, \tag{8.58}$$

$$e^{-2K} = 0. \tag{8.59}$$

where $K = J/kT$. Usually T_c is defined as the value for T for which the correlation length is infinite, therefore, it is considered that $T_c = 0$. In the light of (8.59), it is sensible to define the reduced temperature by

$$\begin{aligned} t &= e^{-2K}, \\ &= e^{-2J/kT}. \end{aligned} \tag{8.60}$$

where K is J/kT. Now that the value for t is found, all the critical exponents can be evaluated. When $h = 0$ both the eigenvectors can be found.

$$\begin{aligned} \lambda_1 &= e^K \cosh h + \sqrt{e^{2K} \sinh^2 h + e^{-2K}}, \\ &= e^K + e^{-K}, \\ &= 2 \cosh K, \end{aligned} \tag{8.61}$$

Similarly, λ_2 equals

$$\lambda_2 = 2 \sinh K, \tag{8.62}$$

Substituting the above results in (8.56) yields

$$\xi = \left[\ln \left(\frac{1+t}{1-t} \right) \right] \tag{8.63}$$

Letting t to be much smaller than one and Taylor expanding the logarithmic terms gives

$$\xi \sim (2t)^{-1}. \tag{8.64}$$

This simplification is justified by the critical behaviour of the correlation length which is of the form, $\xi \sim |t|^{-\nu}$, therefore, the first critical exponent ν is found to be equal to

$$\nu = 1. \tag{8.65}$$

Next, substituting the reduced temperature (8.60) in the expression for magnetisation (8.31) gives

$$m(H,T) = \frac{t^{-1/2}\sinh h}{t^{-1/2}\sqrt{\sinh^2 h + t^2}}, \tag{8.66}$$

Taylor expanding the term sinh yields

$$m(H,T) = \frac{h}{\sqrt{h^2+t^2}}. \tag{8.67}$$

Letting temperature approaches the critical temperature, the expression for magnetisation becomes constant and comparing this situation with (5.1) yields δ to be infinite:

$$\delta = \infty. \tag{8.68}$$

Recalling (8.67)

$$m(H,T) = \frac{h}{h\sqrt{1+t^2/h^2}}. \tag{8.69}$$

Letting $t = 0$, the magnetisation becomes one, i.e,

$$m(H,T) = 1 \tag{8.70}$$

Comparing the above expression for magnetisation with (3.1) yields another critical exponent 'β' to be

$$\beta = 0. \tag{8.71}$$

Next in order to find the value for the critical exponent γ, differentiating the expression (8.31) with respect to reduced external field h gives

$$\begin{aligned}
\chi(H,T) &= \frac{e^K \cosh h[e^{2K}\sinh^2 h + e^{-2K}]^{1/2} - e^{3K}\sinh^2 h \cosh h[e^{2K}\sinh^2 h + e^{-2K}]^{1/2}}{[e^{2K}\sinh^2 h + e^{-2K}]}, \\
&= \frac{e^K \cosh h[e^{2K}\sinh^2 h + e^{-2K} - e^{2K}\sinh^2 h]}{[e^{2K}\sinh^2 h + e^{-2K}]^{3/2}]}, \\
&= \frac{e^{-K}\cosh h}{[e^{2K}\sinh^2 h + e^{-2K}]^{3/2}}.
\end{aligned} \tag{8.72}$$

Letting $h = 0$ and using (8.60), the above expression becomes

$$\begin{aligned} \chi &= \frac{e^{-K}}{e^{-3K}}, \\ &= t^{-1}. \end{aligned} \tag{8.73}$$

This formulation gives the critical behaviour of susceptibility, where $\chi \sim |t|^{-\gamma}$, showing the value of γ to be one.

$$\gamma = 1. \tag{8.74}$$

The naive expression for the specific heat

$$C = \frac{\partial e}{\partial T}. \tag{8.75}$$

would lead to a value for the exponent α which is inconsistent with the scaling relations. But since the reduced temperature is defined as in (8.60) it is more sensible to define specific heat as a derivative with respect to t (Campbell 2008). In fact, from section 7, one has

$$f \sim t^{2-\alpha}. \tag{8.76}$$

Now, letting $h = 0$ the expression for the free energy (8.27) becomes

$$\begin{aligned} f &= -kT \ln[e^K + e^{-K}], \\ &= -kT \left[\ln e^K + \ln(1 + e^{-2K})\right], \\ &= -kT[K + \ln(1 + t)], \\ &\sim \ln(1 + t), \end{aligned} \tag{8.77}$$

Using the taylor expansion, this can be written as

$$f \sim t^1 - \frac{1}{2}t^2 + \cdots. \tag{8.78}$$

Comparing (8.76) and (8.78) gives the critical exponent α to be

$$\alpha = 1. \tag{8.79}$$

Having calculated all the exponents as depicted in the following table, all the scaling relations corresponding to these exponents are now satisfied.

Thermodynamics functions	Behaviour	d=1
Specific Heat	$C \sim \|t\|^{-\alpha}$	$\alpha = 1$
Spontaneous Magnetisation	$M \sim (t)^{\beta}$	$\beta = 0$
Susceptibility	$\chi \sim \|t\|^{-\gamma}$	$\gamma = 1$
Magnetisation	$M \sim H^{\frac{1}{\delta}}$	$\delta = \infty$
Correlation Length	$\xi \sim \|t\|^{-\nu}$	$\nu = 1$

Table 8.1: Critical exponents in one-dimensional Ising model

9 Mean Field Theory

Approaches to Mean Field Theory

The solution for any system consisting of multiple bodies is beyond easy calculation - it is almost impossible to calculate the exact value of partition function for non-trivial models, for instance, certain two or three-dimensional models (Yeomans 1997). This necessitates the introduction of mean field theory (MFT) which involves an average interaction of all neighbouring bodies instead of individual interactions. Thus, MFT gives an approximation for such cases. Furthermore, there are various ways to generate this approximation, for example, Landau theory (Dobrosavljevic 2005), Bogoliubov Inequality (Callen 1985) and Van der Waals approach (Dobrosavljevic 2005). However, the three approaches, Bragg-Williams (Baxter 2007), Weiss MFT (Ravndal 1976) and Saddle Point Solution (Dobrosavljevic 2005), are outlined in this section. The idea behind this theory is to analyze the properties of the previously discussed model of a magnet and then chronologically examine the behaviour of all the thermodynamic functions.

Bragg-William's Approximation

In 1934, Bragg and Williams investigated the Ising model in infinite dimensions. The idea behind this approach is that it allows the spins to interact with all the other spins. As a result, the total energy of the system (4.5) can now be altered by breaking the first term into two parts:

$$\sum_i s_i \left(-J \sum_{j=1}^{q} s_j \right), \tag{9.1}$$

where the summation is over the q sites which interacts with the site i. Using this idea, if there are N sites in a system then the number of possible interaction will be $(N-1)$. However, in (4.5) the summation is over the nearest neighbour i.e, there are $(N-1)/q$ extra sites. In order to balance, divide the above expression by $(N-1)/q$. Consequently,

the above expression takes the form

$$-Jq(N-1)^{-1}\sum_{j=1}^{N-1} s_j. \tag{9.2}$$

Substituting this into (4.5) gives

$$\begin{aligned} E_T &= \sum_i s_i \left(-Jq(N-1)^{-1}\sum_{j=1}^{N-1} s_j\right) - H\sum_i s_i, \\ &= -Jq(N-1)^{-1}\sum_{i,j,i\neq j} s_i s_j - H\sum_i s_i. \end{aligned} \tag{9.3}$$

The above equation is the expression for the total energy of the system. Since each spin interacts equally with all the other spins, therefore, the system is in infinite dimensions. Now squaring both the sides of (4.6) gives

$$M^2 = \left(\sum_{i=1}^{N} s_i\right)^2, \tag{9.4}$$

$$\begin{aligned} &= (s_1+s_2+s_3+\cdots+s_N)^2, \\ &= (s_1^2+s_1s_2+s_1s_3+\cdots+s_1s_N+s_2s_1+s_2^2+s_2s_3+\cdots+s_2s_N+\cdots+s_N^2), \\ &= s_1^2+s_2^2+\cdots+s_N^2+2(s_1s_2+s_1s_3+\cdots+s_1s_N+s_2s_3+\cdots+s_2s_N+\cdots), \\ &= \sum_i^N s_i^2 + 2\sum_{i,j,i\neq j} s_i s_j. \end{aligned} \tag{9.5}$$

Since, s_i takes only two values i.e., ± 1, therefore, squaring either $+1$ or -1 will be positive only. As a result, the above equation becomes

$$M^2 = \sum_i^N 1 + 2\sum_{i,j,i\neq j} s_i s_j.$$

Therefore,

$$\frac{1}{2}(M^2-N) = \sum_{i,j,i\neq j} s_i s_j. \tag{9.6}$$

Substituting the above expression in (9.3) yields

$$E_T = \frac{-Jq}{2}(N-1)^{-1}(M^2-N) - HM. \tag{9.7}$$

Consider N spins in a system and let r spins be pointing downward (i.e, have value -1) then the number of spins pointing upward is $N-r$. Thus, the magnetisation which is

equal to the total spins pointing upward (i.e, $N-r$) minus the spins pointing downward (i.e, r) becomes

$$\begin{aligned} M &= (N-r)-r, \\ &= N-2r. \end{aligned} \tag{9.8}$$

There are N_{C_r} arrangements for the spins;

$$N_{C_r} = \frac{N!}{r!(N-r)!}. \tag{9.9}$$

Substituting (9.8) and (9.9) in (4.11) gives an expression for the partition function. I.e.,

$$Z = \sum_{r=0}^{N} \left(\frac{N!}{r!(N-r)!} e^{\frac{1}{2}\beta Jq([N-2r]^2-N)/(N-1)+\beta H(N-2r)} \right), \tag{9.10}$$

$$= \sum_{r=0}^{N} c_r. \tag{9.11}$$

where

$$c_r = \frac{N!}{r!(N-r)!} e^{\frac{1}{2}\beta Jq([N-2r]^2-N)/(N-1)+\beta H(N-2r)}. \tag{9.12}$$

Next replacing M by $N-2r$ in (4.8), simplifies the magnetisation to give

$$\begin{aligned} m &= \frac{1}{N}\frac{1}{Z}\sum_{r=0}^{N}(N-2r)e^{-\beta E}, \\ &= \frac{1}{Z}\sum_{r=0}^{N}(1-2r/N)e^{-\beta E}. \end{aligned} \tag{9.13}$$

Substituting the expression for the total energy gives

$$m = \frac{1}{Z}\sum_{r=0}^{N}(1-2r/N)e^{\frac{1}{2}\beta Jq([N-2r]^2-N)/(N-1)+\beta H(N-2r)}. \tag{9.14}$$

Since this concept relates to the interaction of all the spins and the above expression does not compute the possible arrangement of the spins so this must be modified to give

$$m = \frac{1}{Z}\sum_{r=0}^{N}(1-2r/N)\frac{N!}{r!(N-r)!}e^{\frac{1}{2}\beta Jq([N-2r]^2-N)/(N-1)+\beta H(N-2r)}, \tag{9.15}$$

Using c_r as in (9.12) gives an expression for an average magnetisation per site:

$$m = \frac{1}{Z}\sum_{r=0}^{N}\left(1-\frac{2r}{N}\right)c_r. \tag{9.16}$$

Now consider the relation $d_r = c_{r+1}/c_r$ by which it is possible to observe the behaviour of c_r at different values of N. Using (9.12), d_r is written as

$$\begin{aligned} d_r &= \frac{c_{r+1}}{c_r}, \qquad (9.17)\\ &= \frac{\frac{N!}{(r+1)!(N-r-1)!}e^{\frac{1}{2}\beta qJ([N-2(r+1)]^2-N)/(N-1)+\beta H(N-2[r+1])}}{\frac{N!}{r!(N-r)!}e^{\frac{1}{2}\beta qJ([N-2r]^2-N)/(N-1)+\beta H(N-2r)}},\\ &= \frac{(N-r)}{(r+1)}\left[e^{\frac{1}{2}\beta qJ(([N^2+4(r+1)^2-4N(r+1)]-N-[N^2+4r^2-4Nr]+N)/(N-1))+\beta H(N-2r-2-N+2r)}\right],\\ &= \frac{(N-r)}{(r+1)}e^{\frac{1}{2}\beta qJ(4N-8r-4)/(N-1)-2\beta H},\\ &= \frac{(N-r)}{(r+1)}e^{-2\beta qJ\frac{(N-2r-1)}{(N-1)}-2\beta H}. \qquad (9.18) \end{aligned}$$

Once the expression for d_r is found, substitute the different values of r i.e., from $0 \cdots N$ in order to see the behaviour of d_r. Therefore, when r equals zero

$$d_0 = Ne^{-2\beta qJ-2\beta H}. \qquad (9.19)$$

Similarly, when r equals $N-1$, d_r becomes

$$d_{N-1} = N^{-1}e^{2\beta qJ-2\beta H}. \qquad (9.20)$$

It can be seen from the above formulation that right hand side increases from order N (maximum value) to order N^{-1} (minimum value) when different values of r, increasing from 0 to $N-1$, are substituted. Now making an assumption that d_r decreases, when r goes from 0 to $(N-1)$, monotonically. There should be a value r_0 such that the condition $d_{r_0} \approx 1$ holds true. The relation of d_r as given in (9.17) can be written as

$$d_r c_r = c_{r+1}. \qquad (9.21)$$

When $d_r > 1$ then c_{r+1} is greater than c_r and the c_r's increases as r goes from 0 to $r_0 - 1$. On the other side when d_r is less than 1, then $c_{r+1} < c_r$ and the c_r's are decreasing when r equals $r_0 + 1 \cdots N$. Since the largest value of c_r relates to the point r_0, c_{r_0} is therefore maximum. Taking $N \to \infty$ then d_r can be written as

$$d_r = \frac{1-\frac{r}{N}}{\frac{r}{N}}e^{-2\beta qJ(1-2r/N)-2\beta H}. \qquad (9.22)$$

Letting $1 - 2r/N$ be x gives

$$\begin{aligned} d_r &= \frac{1 - \frac{1}{2}(1-x)}{\frac{1}{2}(1-x)} e^{-2\beta qJx - 2\beta H}, \\ &= \frac{1+x}{1-x} e^{-2\beta qJx - 2\beta H}. \end{aligned} \tag{9.23}$$

which can be equivalently written as a function of x;

$$d_r = \phi(x). \tag{9.24}$$

which means that $d_r = 1$ corresponds to $\phi(x) = 1$. Now let x_0 be the solution of the equation $\phi(x) = 1$. Next assuming that c_{r_0} dominates all the other c_r which means that in this approach all the other c_r's are assumed to be negligible. Using this assumption, the partition function can now be expressed as

$$Z \approx c_{r_0}. \tag{9.25}$$

Magnetisation

Further, in order to obtain the expression for magnetisation, substituting the above expression in (9.16) gives

$$m = 1 - \frac{2r_0}{N}. \tag{9.26}$$

which can be equivalently written as

$$m = x_0. \tag{9.27}$$

Since, x_0 is given by $\phi(x_0) = 1$, in the same way m is given by $\phi(m) = 1$. This means the expression (9.23) can be written as

$$1 = \frac{1+m}{1-m} e^{-2\beta qJm - 2\beta H}. \tag{9.28}$$

Rearranging the above gives a simplified version of magnetisation

$$1 - e^{-2\beta(qJm+H)} = m(e^{-2\beta(qJm+H)} + 1),$$

$$m = \frac{1 - e^{-2\beta(qJm+H)}}{1 + e^{-2\beta(qJm+H)}},$$

$$m = \tanh[(qJm + H)/kT]. \tag{9.29}$$

The above equation is an expression for magnetisation as a function of H and T. This was first developed in 1934 by Bragg and Williams.

Free Energy

Using (9.12), the expression for the free energy f can be obtained. Substituting (9.25) in (4.15) gives

$$f = \lim_{N\to\infty} \frac{1}{N} \ln c_{r_0}. \tag{9.30}$$

Now, using Stirling's approximation:

$$n! \sim (2\pi)^{1/2} e^{-n} n^{n+1/2} \tag{9.31}$$

Equation (9.12) becomes

$$c_{r_0} = \frac{N^{N+1/2}}{(2\pi)^{1/2} {r_0}^{r_0+1/2} (N-r_0)^{N-r_0+1/2}} e^{\frac{1}{2}\beta qJ([N-2r_0]^2-N)/(N-1)+\beta H(N-2r_0)}. \tag{9.32}$$

Substituting the above expression into (9.30), the free energy can be written as

$$\begin{aligned} f &= \frac{1}{N}\left[\ln(N^{N+1/2}) - \ln(2\pi)^{1/2} - \ln(r_0)^{r_0+1/2} - \ln(N-r_0)^{N-r_0+1/2}\right] + \\ &\quad \frac{1}{N}\left[\frac{1}{2}\beta qJ[(N-2r_0)^2 - N]/(N-1) + \beta H(N-2r_0)\right], \\ &= \left(1+\frac{1}{2N}\right)\ln N - \frac{1}{2N}\ln 2\pi - \left(\frac{r_0}{N}+\frac{1}{2N}\right)\ln r_0 - \left(1-\frac{r_0}{N}+\frac{1}{2N}\right)\ln(N-r_0) \\ &\quad + \frac{1}{2}\beta qJ\left[\frac{(1-\frac{2r_0}{N})^2 - \frac{1}{N}}{1-\frac{1}{N}}\right] + \beta H\left[1-\frac{2r_0}{N}\right]. \end{aligned} \tag{9.33}$$

As N approaches to infinity, the constant terms and terms like $1/2N$, $1/N$ will not be considered and using the relationship $m = 1 - 2r_0/N$, the free energy becomes

$$\begin{aligned} f &= \ln N - \frac{1}{2}(1-m)\ln\left(\frac{N(1-m)}{2}\right) - \left(1-\frac{1}{2}(1-m)\right)\ln\left(N - \frac{N}{2}(1-m)\right) + \\ &\quad \frac{1}{2}\beta qJm^2 + \beta Hm, \\ &= \ln N - \frac{1}{2}(1-m)\left[\ln N + \ln\left(\frac{1-m}{2}\right)\right] - \frac{1}{2}(1+m)\left[\ln N + \ln\left(\frac{1+m}{2}\right)\right] + \\ &\quad \frac{1}{2}\beta qJm^2 + \beta Hm, \end{aligned}$$

$$
\begin{aligned}
&= -\frac{1}{2}(1-m)\ln\left(\frac{1-m}{2}\right) - \frac{1}{2}(1+m)\ln\left(\frac{1+m}{2}\right) + \frac{1}{2}\beta qJm^2 + \beta Hm, \\
&= -\frac{1}{2}\left[\ln\left(\frac{1-m^2}{4}\right) + m\ln\left(\frac{1+m}{1-m}\right)\right] + \frac{1}{2}\beta qJm^2 + \beta Hm, \qquad (9.34)
\end{aligned}
$$

Using the hyperbolic function $\tanh^{-1}$ in the second logarithm term yields

$$f = -\frac{1}{2}\ln\left(\frac{4}{1-m^2}\right) - m\tanh^{-1} m + \frac{1}{2}\beta qJm^2 + \beta Hm, \qquad (9.35)$$

Next, substituting the expression for $\tanh^{-1} m$ from (9.29) in the above formulation gives

$$f = \frac{1}{2}\ln\left(\frac{4}{1-m^2}\right) - \frac{1}{2}\beta qJm^2. \qquad (9.36)$$

The above equation is an expression for the free energy f as a function of m and T.

Rewrite the equation (9.29) as a function of m and T for H:

$$H = -qJm + kT\tanh^{-1} m. \qquad (9.37)$$

Once the expression for H is obtained then it is possible to construct the graph of H in terms m and vice-versa. In order to do that first consider the constant terms, q, J and k,. Setting each single term to unity, only stretches or compresses the graph, however, the shape of the graph remains the same regardless of the value for the respective terms. In other words, to observe the behaviour of functions H, m and T the constant terms can be set to unity and easily a graph can be constructed i.e, of function $H = -m + \tanh^{-1} m$. However, there still exist three terms in the expression which means if a graph of m is plotted against H then the variable T is left. Therefore, to examine the expression for T, setting external field to zero in (9.37) gives

$$0 = -qJm + kT\tanh^{-1} m. \qquad (9.38)$$

Since $H = 0$, m is called spontaneous magnetisation and is denoted by m_0. Rearranging the expression (9.38) and changing m to m_0 gives

$$m_0 = \tanh\left(\frac{qJm_0}{kT}\right). \qquad (9.39)$$

Now if m_0 is small. Using a Taylor expansion the above expression can be written as

$$m_o = \frac{qJm_0}{kT} + O(m_0^2). \qquad (9.40)$$

As a result,

$$\frac{qJ}{kT} = 1, \tag{9.41}$$

Rearranging the above expression to give T

$$T = \frac{qJ}{k}, \tag{9.42}$$

and when the temperature T approaches critical temperature T_c, the above expression becomes

$$T_c = \frac{qJ}{k}. \tag{9.43}$$

Since in one-dimensional model, spins interact only with the nearby neighbours i.e, $q = 2$. Therefore, using (9.43) the critical temperature for $d = 1$ will be given by $T_c = 2J/k$. However, the critical temperature for one-dimensional model equals zero. As a result, this shows that MFT is not true for atleast $d = 1$.

Setting constant terms to one in (9.37), there exists three scenarios for T which need to be considered. These are

$$T = T_c, \quad T > T_c \quad \text{and} \quad T < T_c. \tag{9.44}$$

Thus, the graph of m against H can be constructed. Figure 9.1 illustrates that when temperature equals critical temperature the magnetistaion vanishes which means as the temperature approaches to critical temperature the system gets demagnetised.

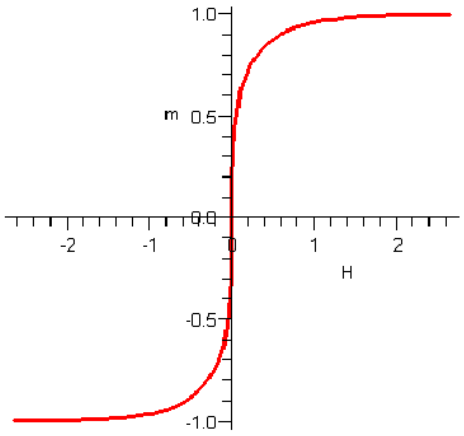

Figure 9.1: The graph of m as a function of H when $T = T_c$

On the other hand when the temperature is increased further and is more than the critical temperature, depicts that the system remains to be same as continuous but the graph founds to be more extended and stretched. This scenario when $T > T_c$ is shown in figure 9.2

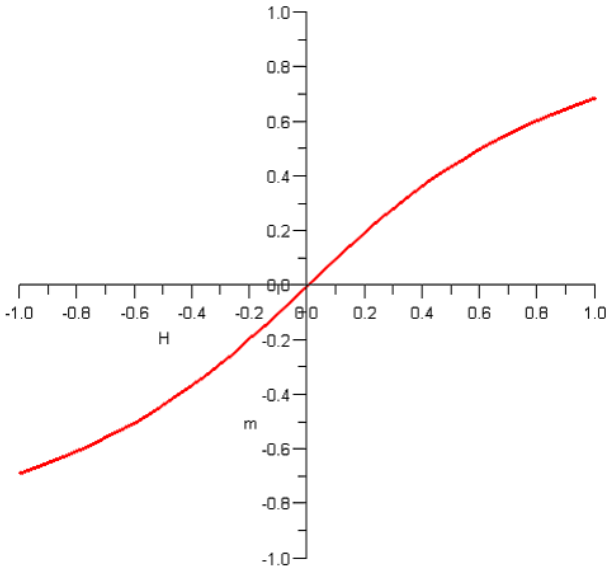

Figure 9.2: The graph of m as a function of H when $T > T_c$

The third graph illustrated in figure 9.3 depicts the relationship of magnetisation and H when the temperature is below the critical temperature.

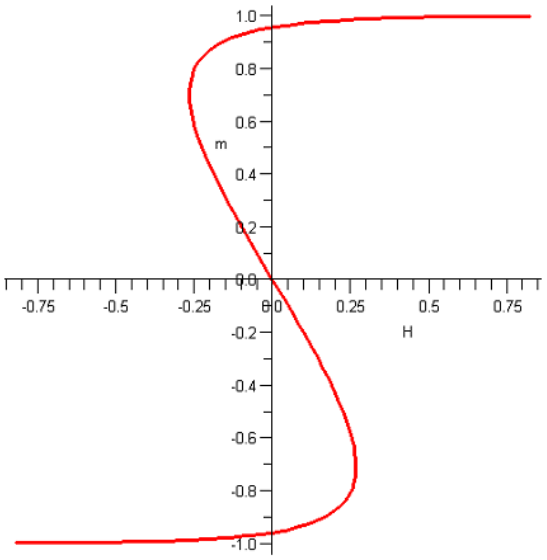

Figure 9.3: The graph of m as a function of H when $T < T_c$

However, this graph gives three values for the magnetsiaion in the absence of external magnetic field which is not valid as the magnetisation can take only one value at one time. The reason behind this contradiction is the assumption which was made in expression (9.18) because if temperature is less than T_c than it can be seen from (9.18) that d_r is not monotonically decreasing and the function c_r instead of c_{r_0} maximum will now have two maximum points. In order to correct this contradiction a new graph can be constructed showing only one value for the magnetisation.

Now using the above expressions for magnetistaion and the free energy, the critical exponents can be found. In order to do that, substitute (9.43) in the expression for the reduced temperature (3.2) gives

$$t = \frac{kT - qJ}{qJ}. \tag{9.45}$$

which can also be written as

$$\begin{aligned} kT &= tqJ - qJ, \\ T &= \frac{qJ}{k}(t+1). \end{aligned} \tag{9.46}$$

Substituting the equation for T in (9.39) yields

$$\begin{aligned} \tanh^{-1} m_0 &= \frac{qJm_0}{qJ(t+1)}, \\ m_0 &= (t+1)\tanh^{-1} m_0. \end{aligned} \tag{9.47}$$

When $T > T_c$, the spontaneous magnetisation is small. Taylor expanding the hyperbolic function tanh gives

$$\tanh^{-1} m_0 = m_0 + \frac{m_0^3}{3} + \frac{m_0^5}{5} + \frac{m_0^7}{7} + \cdots, \tag{9.48}$$

Since m_0 is small therefore the higher than three terms can be considered negligible and the expansion tanh can be written as

$$\tanh^{-1} m_0 \approx m_0 + \frac{m_0^3}{3}. \tag{9.49}$$

Substituting this in (9.47) gives

$$m_0 = (t+1)\left(m_0 + \frac{m_0^3}{3}\right),$$

$$m_0 = \sqrt{\frac{-3t}{t+1}}, \tag{9.50}$$

which can also be written as

$$m_0 = (-3t)^{1/2}(1+t)^{1/2}. \tag{9.51}$$

Next Taylor expanding $(1+t)^{1/2}$ gives

$$(1+t)^{1/2} = 1 - \frac{t}{2} + \frac{3t^2}{8}\cdots, \tag{9.52}$$

The above expansion will be considered to order t because near the critical temperature T_c, the reduced temperature is zero. As a result, equation (9.51) can now be written as

$$m_0 = (-3t)^{1/2}\{1 + O(t)\}. \tag{9.53}$$

where $O(t)$ is the terms of order t. Now considering $T < T_c$ and comparing the above expression with (3.1) gives

$$m_0 = (-t)^{1/2}. \tag{9.54}$$

and the first critical exponent β is given by

$$\beta = 1/2. \tag{9.55}$$

Now in order to evaluate the free energy and the critical exponent α consider the scenario $T > T_c$. If H approaches zero then $m \to 0$. The free energy (9.36) can be expressed as

$$\begin{aligned} \frac{-f}{kT} &= \frac{1}{2}\ln[4], \\ -f/kT &= \ln 2. \end{aligned} \tag{9.56}$$

Diiferentiating twice the free energy with respect t equals zero in this case. On the other side, m approaches to m_0 when $T < T_c$. Substituting this in the free energy (9.36) gives

$$f/kT = \ln 2 - \frac{1}{2}\ln(1 - m_0^2) - \frac{1}{2}\frac{qJm_0^2}{kT}, \tag{9.57}$$

Next, using Taylor expansion and substituting the expression for the temperature and spontaneous magnetisation gives

$$\begin{aligned} f/kT &= \ln 2 - \frac{3t}{2(1+t)}\left(1 - \frac{1}{1+t}\right) + \frac{9}{4}\frac{t^2}{(1+t)^2} - \frac{9}{4}\frac{t^3}{(1+t)^3} + O(t^4), \\ &= \ln 2 - \frac{3t^2}{2(1+t)^2} + \frac{9}{4}\frac{t^2}{(1+t)^2} - \frac{9}{4}\frac{t^3}{(1+t)^3} + O(t^4), \\ &= \ln 2 + \frac{3}{4}\frac{t^2}{(1+t)^2} - \frac{9}{4}\frac{t^3}{(1+t)^3} + O(t^4), \end{aligned} \tag{9.58}$$

Now $1/(t+1) \to 1$ if t is small and negative which means

$$f/kT = \ln 2 + \frac{3}{4}t^2 - \frac{9}{4}t^3 + O(t^4). \tag{9.59}$$

As mentioned in (4.21), the specific heat is mathematically defined as the second derivative of the free energy with respect to β. Differentiating the above equation with respect to reduced temperature gives

$$f' = \frac{3}{2}t - \frac{27}{4}t^2, \tag{9.60}$$

$$f'' = \frac{3}{2} - \frac{27}{2}t. \tag{9.61}$$

which can also be written in terms of order t i.e,

$$f'' = C = \frac{3}{2}t^0 + O(t). \tag{9.62}$$

From the above expression for the free energy (9.56) and (9.59), it can be observe that the free energy at critical temperature is continuous, however, the specific heat shows a discontinuity because specific heat is zero at $t < 0$ and is equal to $3/2$ when $t > 0$. Hence, it displays discontinuity and does not justify the behaviour of specific heat $c \sim |t|^{-\alpha}$ which implies the critical exponent 'α' to be zero, i.e,

$$\alpha = 0. \tag{9.63}$$

Next in order to find the value for the critical exponent γ, differentiate the expression (9.37) with respect to external field 'H', keeping T fixed.

$$1 = -qJ\frac{\partial m}{\partial H} + kT\frac{1}{1-m^2}\frac{\partial m}{\partial H},$$

$$\frac{\partial m}{\partial H} = \frac{1-m^2}{-qJ(1-m^2)+kT}. \tag{9.64}$$

Replacing T by (9.46) gives

$$\frac{\partial m}{\partial H} = \frac{1-m^2}{qJ(t+m^2)}. \tag{9.65}$$

The susceptibility is the first derivative of magnetisation with respect to external field, therefore, the above expression yields

$$\chi = \frac{1-m^2}{qJ(t+m^2)}. \tag{9.66}$$

Next consider the scenario when $T > T_c$. In the absence of external field, the magnetisation approaches zero. Therefore, the above expression becomes

$$\chi = \frac{1}{qJt}. \tag{9.67}$$

On the other side, if temperature is less than critical temperature then m approaches m_0 and susceptibility in (9.66) is written as

$$\chi^{-1} = -qJ + \frac{kT}{1 - m_0^2}, \tag{9.68}$$

Substituting the value for spontaneous magnetisation (9.50) and using the taylor expansion, the susceptibility becomes

$$\begin{aligned} \frac{\chi^{-1}}{kT_c} &= \frac{1}{T_c}\left[-T_c + T(1 - 3t + (3t)^2 \cdots)\right], \\ &= \frac{T - T_c}{T_c} - \frac{3T}{T_c}t + \frac{9T}{T_c}t^2 \cdots, \\ &= t - \frac{3T}{T_c}t + \frac{9T}{T_c}t^2 \cdots, \end{aligned} \tag{9.69}$$

Using (9.43) and (9.46), the above expansion can be written as

$$\chi^{-1} = qJ(-2t + 6t^2 + 9t^3 \cdots), \tag{9.70}$$

or

$$\chi = (-2tqJ)^{-1}[1 - 3t - 9/2t^2 \cdots]^{-1}, \tag{9.71}$$

Near the critical temperature the expansion is of order t, therefore, the susceptibility becomes

$$\chi = (-2tqJ)^{-1}[1 + 3t], \tag{9.72}$$

and when t is small then χ approximately equivalent to

$$\chi \approx (-2tqJ)^{-1}. \tag{9.73}$$

Recalling the behaviour of the susceptibility as in (5.4) and comparing with (9.67) and (9.73) gives the critical exponent γ as

$$\gamma = 1. \tag{9.74}$$

Using (9.37) and taylor expanding the hyperbolic function $\tanh^{-1}$, the last critical exponent δ can be obtained.

$$H = -qJm + kT\left(m + \frac{m^3}{3} + \frac{m^5}{5} + \frac{m^7}{7} + \cdots\right), \tag{9.75}$$

Substituting (9.46) in the above expression gives

$$H = -qJm + qJ(t+1)\left(m + \frac{m^3}{3} + \frac{m^5}{5} + \frac{m^7}{7} + \cdots\right),$$

$$\frac{H}{kT_c} = tm + t\frac{m^3}{3} + t\frac{m^5}{5} + t\frac{m^7}{7} + \frac{m^3}{3} + \frac{m^5}{5} + \frac{m^7}{7}. \tag{9.76}$$

Setting reduced temperature to be zero yields

$$\frac{H}{kT_c} = \frac{m^3}{3} + \frac{m^5}{5} + \frac{m^7}{7}, \tag{9.77}$$

The terms of higher order than three are negligible if m is small. Thus, the above expansion can now be written as

$$\frac{H}{kT_c} = \frac{m^3}{3}, \tag{9.78}$$

which implies

$$H \sim m^3. \tag{9.79}$$

Comparing this with (5.1) gives the critical exponent δ

$$\delta = 3. \tag{9.80}$$

Finally, all the critical exponents are examined above except the correlation length because according to this approach every spin interacts with all other spins and there is no description about the location of spins. Thus, the exponents ν, η and μ are not defind for this theory. However there is another approach called thehigh temperature series expansion which can be used to find the remaining exponents. This approach is been elaborated in a later section.

Weiss MF Theory

Weiss MF is another approach to solve Ising model. Historically this technique was invented by P. E. Weiss (1865-1940) as a theory of magnetism. The underlying assumption of Weiss theory is to assume that energy of the system can be represented by an average external field, H_W, acting on the spins.

$$H_W = \lambda m, \tag{9.81}$$

where H_W is denoted by the average external field and the total magnetic field H_T enacting on all the spins is then given by the sum of initial magnetic field plus the Weiss assumption, which is

$$H_T = H + \lambda m. \tag{9.82}$$

Replacing the external magnetic field by equation (9.82) and β in the definition of reduced magnetic field i.e.,

$$h = \frac{H + \lambda m}{kT}. \tag{9.83}$$

If the spins in the system have no interaction with each other then the energy equals zero. From (4.14), the partition function takes the form

$$Z = \sum_{\{s_i\}} e^{hM}. \tag{9.84}$$

where h is the reduced external field as in (9.83). Now substituting the expression for M and expanding the summation s_i by using the properties of exponentials gives

$$\begin{aligned} Z &= \sum_{\{s_i\}} e^{h\sum_{i=1}^{N} s_i}, & (9.85)\\ &= \sum_{\{s_i\}} e^{hs_1}.e^{hs_2}.e^{hs_3}\cdots, & (9.86) \end{aligned}$$

The spin at site i takes only two values ± 1, therefore, this becomes

$$\begin{aligned} Z &= \sum_{\{s_i\}} e^{h(\pm 1)} e^{h(\pm 1)} e^{h(\pm 1)} e^{h(\pm 1)} \cdots, & (9.87)\\ &= (e^h + e^{-h})(e^h + e^{-h})(e^h + e^{-h})(e^h + e^{-h})\cdots, \end{aligned}$$

which is

$$Z = \prod_N (e^h + e^{-h}), \tag{9.88}$$

Using the hyperbolic function for cosh, the partition function becomes

$$Z = \prod_N (2\cosh(h)), \tag{9.89}$$

which is equivalent to

$$Z = (2\cosh(h))^N. \tag{9.90}$$

The next step is to determine the magnetisation of the system which is defined as the negative first derivative of the free energy in terms of external field H. Recalling the expression for the free energy (4.15) and substituting the partition function (9.90) yields

$$f = -kT\frac{1}{N}\ln(2\cosh(h))^N, \tag{9.91}$$

$$= -kT\ln(2\cosh(h)). \tag{9.92}$$

Differentiating the free energy with respect to reduced external field and replacing h by (9.83), gives magnetisation

$$m = \tanh\left(\frac{H + \lambda m}{kT}\right). \tag{9.93}$$

In the absence of external field, the magnetisation of the system becomes

$$m = \tanh\left(\frac{\lambda m}{kT}\right), \tag{9.94}$$

This can be represented graphically by plotting both the curves in terms of their coordinates. This has been illustrated in Figure 9.4.

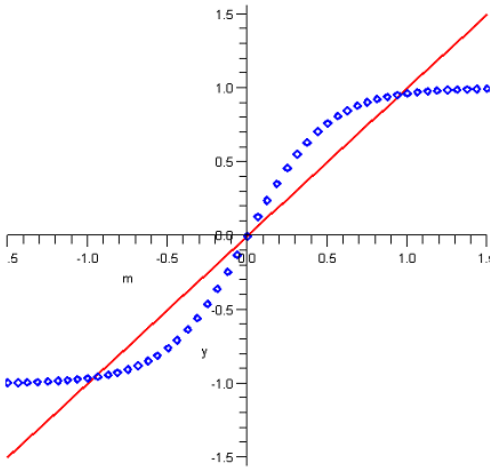

Figure 9.4: The graphical solution to $m = \tanh\left(\frac{\lambda m}{kT}\right)$ in the absence of external field.

Now making an assumption that m is small and temperature approaches the critical temperature T_c, using taylor expansion on tanh gives

$$m \approx \frac{\lambda m}{kT_c}, \tag{9.95}$$

This gives an expression for the critical temperature:

$$T_c = \frac{\lambda}{k}. \tag{9.96}$$

Next, in the presence of external field the expression for magnetisation, using (9.96), can be written as

$$\begin{aligned} m &= \tanh\left(\frac{H}{kT} + \frac{\lambda m}{kT}\right), \\ &= \tanh\left(\frac{H}{kT} + \frac{T_c m}{T}\right). \end{aligned} \tag{9.97}$$

If T_c/T is denoted by the variable x, then magnetisation can be rewritten as

$$m = \tanh\left(\frac{H}{kT} + mx\right). \tag{9.98}$$

The above equation is the expression for the magnetisation which recovers the equation of Bragg-William's (9.29). As a result, one can find the critical exponents β, γ and δ using the similar procedure as used earlier. Since both the expressions are equal, therefore, they share the same values for the critical exponents, as listed below:

$$\beta = \frac{1}{2}, \quad \gamma = 1 \quad \text{and} \quad \delta = 3.$$

However, the other critical exponent α can be analyzed by replacing h in (9.92) by (9.83).

$$f = -kT \ln\left(2\cosh\left(\frac{H + \lambda m}{kT}\right)\right). \tag{9.99}$$

and in the absence of external field the free energy simplifies to

$$f = -kT \ln\left(2\cosh\left(\frac{\lambda m}{kT}\right)\right), \tag{9.100}$$

Next in order to examine the behaviour of the free energy consider two cases i.e, above and below the critical temperature. When temperature is larger than the critical temperature then the magnetisation equals zero and the free energy becomes

$$-f/kT = \ln(2). \tag{9.101}$$

This formulation is similar to the expression for Bragg-William's in (9.56). Further differentiating the above expression of free energy twice yields a specific heat of zero. Now, when the temperature is less than critical temperature, the expression for the free energy, using (9.96), becomes

$$f = -kT \ln\left(2\cosh\left(\frac{T_c m}{T}\right)\right). \tag{9.102}$$

Now, when the temperature approaches the critical temperature, $T \to T_c$, this modifies the above expression to give

$$f = -kT \ln(2\cosh(m)). \tag{9.103}$$

From the Bragg-William's approach, when the temperature was less than the critical temperature, the magnetisation was found to be $t^{1/2}$, therefore, substituting this in (9.103) gives

$$f = -kT \ln(2\cosh(t^{\frac{1}{2}})). \tag{9.104}$$

Finally in order to examine the behaviour of the specific heat, differentiate the free energy in terms of reduced temperature t and then let t equal zero, which yields a non zero value. As a result, it shows a discontinuity when the temperature equals zero and does not satisfy the relationship $C \sim |t|^{-\alpha}$. So the critical exponent 'α' is found to be zero.

Saddle Point Solution

Apart from Bragg and William and Weiss approach, there also exist another approach to MF. Since many assumptions have been made in relation to the MFT, the accuracy of the calculated critical exponents is unclear due to which continuous observations have been carried out to check their reliability. However, it appears that the description of the critical exponents is not necessarily valid (Dobrosavljevic 2005). The overall plan of this section is to re-derive more rigorous expressions for MF by considering the Weiss approach to be exact.

In order to do that, a limit must be identified. At any temperature the spin at site i, takes only two values so it is either positive or negative and has no preferred direction.

This means that the external magnetic field can be stated as the total of N random spins variables. From the definition of elementary statistics " *any sum of random numbers is increasingly well represented by its algebraic average, provided that the number of terms becomes larger and larger*" (Dobrosavljevic 2005), it can be assumed that MF approximation is exact for large N. Next, in order to check how large n should be for the accuracy of MF approach consider the scale of interaction i.e, first set $J \to \frac{J}{N}$ and the limit $N \to \infty$. As a result, MFT becomes exact and free energy becomes finite. Using the assumption, the energy of the system is given by

$$E = -\frac{J}{2N}M^2, \tag{9.105}$$

Substituting the above expression in (4.7), the total energy of the system becomes

$$E_T = -\frac{J}{2N}M^2 - HM. \tag{9.106}$$

The partition function now takes the form:

$$Z = \sum_{\{s_i\}} e^{\frac{\beta J}{2N}M^2 + \beta HM}. \tag{9.107}$$

Next, using the Gaussian identity (see Appendix B)

$$\int_{-\infty}^{\infty} e^{-ax^2+bx+c}dx = e^{\frac{b^2}{4a}+c}\left(\frac{\pi}{a}\right)^{\frac{1}{2}} \tag{9.108}$$

in the first exponential term of (9.107) gives

$$\begin{aligned} e^{\frac{\beta J}{2N}M^2} &= e^{\frac{\beta J}{2N}M^2}\left(\frac{2\beta J\pi}{N}\right)^{\frac{1}{2}}, \\ &= \left(\frac{N}{2\pi\beta J}\right)^{\frac{1}{2}}\int_{-\infty}^{\infty} e^{\frac{-N}{2\beta J}x^2 + Mx}dx. \end{aligned} \tag{9.109}$$

The partition function can then be rewritten as

$$Z = \left(\frac{N}{2\pi\beta J}\right)^{\frac{1}{2}}\int_{-\infty}^{\infty} e^{\frac{-N}{2\beta J}x^2}dx \sum_{\{s_i\}} e^{(\beta H+x)M}dx. \tag{9.110}$$

Letting

$$Z_1 = \left(\sum_{\{s_i\}} e^{(\beta H+x)M}\right)^N, \tag{9.111}$$

and substituting the value for M gives

$$Z_1 = 2\cosh(\beta H + x)^N. \tag{9.112}$$

Substituting this into (9.110) yields

$$\begin{aligned} Z &= \left(\frac{N}{2\pi\beta J}\right)^{\frac{1}{2}} \int_{-\infty}^{\infty} dx(e^{\frac{-N}{2\beta J}x^2} + 2\cosh(\beta H + x)^N), \\ &= \left(\frac{N}{2\pi\beta J}\right)^{\frac{1}{2}} \int_{-\infty}^{\infty} dx(e^{N\left[\frac{-x^2}{2\beta J} + \ln 2 + \ln(\cosh(\beta H + x))\right]}). \end{aligned} \tag{9.113}$$

The saddle point solution can be applied, if the assumption that N approaches infinity is made, i.e., the graph of expression (9.113) has a maximum peak, denoted by $T_{\max}$ and equals βJm. Implementing the method yields

$$f(x, H) = -\frac{x^2}{2\beta J} + \ln 2 + \ln(\cosh(\beta H + x)). \tag{9.114}$$

Differentiating with respect of x gives

$$\frac{\partial}{\partial x} f(x, H) = -\frac{x}{\beta J} + \tanh(\beta H + x). \tag{9.115}$$

Setting this equation to zero and letting $x \to T_{\max}$ gives

$$-\frac{T_{\max}}{\beta J} + \tanh(\beta H + T_{\max}) = 0. \tag{9.116}$$

Next, substituting the value for $T_{\max}$ which is known to be βJm gives

$$-\frac{\beta Jm}{\beta J} + \tanh(\beta H + \beta Jm) = 0, \tag{9.117}$$

which can be equivalently written as

$$m = \tanh(\beta H + \beta Jm). \tag{9.118}$$

The above equation is an expression for magnetisation which is identical to the expression found earlier in the Weiss theory. Thus, the expression of magnetisation can now be used to determine all the critical exponent.

To determine the accuracy, the magnitude of N needs to be known. In the absence

of external magnetic field, the sharp maxima of the equation (9.110) is at $x = 0$ whereas if $H \neq 0$ and finite then the maximum point alters to either left or right. Since the integrand is symmetric, the partition function is an even function of H and the magnetisation in the absence of external field is

$$m = \lim_{H\to 0} \frac{1}{N} \frac{\partial}{\partial \beta H} \ln Z(H) = 0. \tag{9.119}$$

which means the first derivative equals zero at the origin, for an even function. It can be seen from figure 9.2 that for finite N the graph of m against H always passes through origin. That means there is no discontinuity in the graph. Finally, the magnetisation is given below in various limits:

$$\lim_{H\to 0} m = 0 \quad \text{for} \quad N \text{ finite},$$

$$\lim_{N\to\infty} \lim_{H\to 0} m = 0 \quad \text{for} \quad T > T_{\max},$$

$$\lim_{H\to 0} \lim_{N\to\infty} m \neq 0 \quad \text{for} \quad T < T_{\max}.$$

This means that discontinuity occurs when N is infinite. Thus, to prove the accuracy of Weiss approach to MF N should be infinite.

High Temperature Series Expansion

Since the location of the spins is not known, therefore, the remaining critical exponents are not apriori justified for the MF theories discussed above. However, using the high temperature series expansion (HTSE), the remaining exponents can in fact be obtained. In order to do this, the notion of second moment must be introduced. The second moment is denoted by μ and defined as

$$\begin{aligned} \mu_2 &= \sum_{\vec{x}} \vec{x}^2 \langle s(0)s(x)\rangle, \\ &= \sum_i {x_i}^2 \langle s_i s_j\rangle. \end{aligned} \tag{9.120}$$

where x is the lattice spacing. When x approaches zero, the second moment becomes

$$\mu_2 = \int_0^{\xi} d^d x \langle s_0 s_x\rangle x^2,$$

$$
\begin{aligned}
&= \int_0^{\xi} r^{3-\eta} dr D(r/\xi), \\
&= \xi^{4-\eta}, \\
&= \xi^2 \xi^{2-\eta}.
\end{aligned} \tag{9.121}
$$

Using (7.11), the second moment equals

$$\mu_2 = \xi^2 \chi. \tag{9.122}$$

A HTSE is a taylor expansion for an exponential term. Recalling the expression for the partition function (4.14) where $\beta = 1/kT$. If the temperature increases, then β is small and using the taylor expansion, the partition function becomes

$$Z = \sum_{\{s_i\}} \left[1 - \beta E_T + \frac{\beta^2}{2!} E_T^2 + \cdots \right]. \tag{9.123}$$

which turns out to be (Butera and Comi 2002)

$$\chi = 1 + q\beta + (q^2 - q)\beta^2 + (q^3 - 2q^2 + q)\beta^3 + \cdots, \tag{9.124}$$

and the second moment to be

$$\mu_2 = q\beta + 2q^2\beta^2 + (3q^3 - 2q^2 + q)\beta^3 \cdots. \tag{9.125}$$

where q is the number of nearby neighbours and for MFT q equals $2d$ where d is the dimensions of the system. Now, letting $d \to \infty$ gives $q \to \infty$. When q is large, then the higher power terms of q will dominate. I.e.,

$$\chi \to 1 + q\beta + q^2\beta^2 + q^3\beta^3 + \cdots, \tag{9.126}$$

and

$$\mu_2 = q\beta(1 + 2q\beta + 3q^2\beta^2 + \cdots). \tag{9.127}$$

Next, taylor expanding $(1 - q\beta)^{-1}$ gives

$$
\begin{aligned}
(1 - q\beta)^{-1} &= 1 + q\beta + q^2\beta^2 + \cdots, \\
&= \chi.
\end{aligned} \tag{9.128}
$$

and taylor expanding $(1-q\beta)^{-2}$ gives

$$\begin{aligned}(1-q\beta)^{-2} &= 1-2(-q\beta)+\frac{-2-3}{2!}(-q\beta)^2+\cdots, \\ &= 1+2q\beta+3(q\beta)^2\cdots. \end{aligned} \tag{9.129}$$

Substituting the above result into (9.127) yields

$$\mu_2 = q\beta(1-q\beta)^{-2}. \tag{9.130}$$

Rearranging the equation (9.128) gives

$$\begin{aligned}\chi &= \frac{1}{1-q\beta}, \\ &= -\frac{1}{q}\left(\beta-\frac{1}{q}\right)^{-1}, \\ &\approx (\beta-\beta_c)^{-1}. \end{aligned} \tag{9.131}$$

Comparing the above expression with (5.4) gives the value for the critical exponent γ to be one. Similarly, the second moment is

$$\begin{aligned}\mu_2 &\sim (1-q\beta)^{-2}, \\ &= (\beta-\beta_c)^{-2}, \\ &\sim t^{-2}. \end{aligned} \tag{9.132}$$

Substituting this in (9.122) gives

$$\begin{aligned}t^{-2} &= \xi^2\chi, \\ t^{-2} &= t^{-2\nu}t^{-\gamma}, \\ -2 &= -2\nu-\gamma, \\ \nu &= \frac{1}{2}. \end{aligned} \tag{9.133}$$

Thus, the critical exponent ν is now known in MF, using the HTSE.

Mean Field Theory and Scaling Relations

The five critical exponents found are listed below

$$\alpha = 0, \quad \beta = \frac{1}{2},$$

$$\gamma = 1, \quad \delta = 3 \quad \text{and}$$

$$\nu = \frac{1}{2}.$$

Finally, the accuracy of the critical exponents is checked by substituting the values for the critical exponents in four scaling relations.

Griffith's law and Rushbrooke's law are found to be satisfied when the value of α, β, γ and δ are substituted in equations (7.45) and (7.50). Substituting the values of ν and α in Josephson's law (7.8) gives the dimensionality of the system to be four. Since the MF assumption are for dimensions greater and equal to four, this means the Josephson's law fails for $d = 5$ and above.

Finally, the Fisher law (7.13) involves the critical exponent η. Now η cannot be obtained using the methods mentioned above. However, replacing γ and ν in (7.13) by their respective values gives the critical exponent η to be

$$\eta = 0. \tag{9.134}$$

Hence, the mean field theory give accurate results for dimensions greater than four which describes the behaviour of the system near the critical point and also satisfies all the scaling relations in four dimensions.

10 Extended Scaling

One is interested in the scaling behaviour of various thermodynamic functions close to phase transitions. According to the traditional approach, the divergent thermodynamic functions near the critical temperature typically display scaling behaviour in the form of

$$O(T) \approx A_O t^{-\rho}. \tag{10.1}$$

where A_O is a critical amplitude, ρ is a critical exponent and t is the usual reduced temperature (3.2). However, it has been observed that this formulation is justified only close to the critical temperature, T_c and this makes it difficult to analyze data from both numerical simulations and experimental analysis (Barber 1983). For this reason other thermal scaling variables have been considered in the literature.

Inspired by the high-temperature series expansion (HTSE), Campbell, Hukushima and Takayama (2006) recently proposed a new method to extract the scaling behaviour in a manner which is claimed to be superior to the traditional approach. This "extended scaling" approach has been tested in two and three dimensions at temperatures above the phase transition. The central aim of this work is to investigate the efficacy of the extended scaling approach in a variety of circumstances, including dimensions five, six, seven and eight. In particular, Campbell, Hukushima and Takayama (2006) proposed replacing the standard variable t by

$$\tau = \frac{T - T_c}{T} = 1 - \frac{\beta}{\beta_c}. \tag{10.2}$$

In the first half of this section, using the rationale given by Campbell, Hukushima and Takayama (2006) the new scaling variable τ will be shown to be more powerful than the conventional scaling variable t between the lower [1] and the upper critical dimensions [2] by retesting it in the two-dimensional Ising model. The extended scaling scenario for systems below the lower critical dimension is analysed in Katzgraber, Campbell and Hartmann

[1] The lower critical dimension is that below which no phase transition takes place. This is $d = 2$ in the ising case.

[2] The upper critical dimension is that above which MFT applies. This is $d = 4$ in the Ising case as shown in chapter 9.

(2008). In the second half, this scheme will be tested and applied for dimensions greater than four i.e., above the upper critical dimension of the Ising model.
The relationships between the two reduced temperatures are

$$t = \frac{\tau}{1-\tau} = \tau + \tau^2 + \tau^3 + \cdots, \tag{10.3}$$

$$\tau = \frac{t}{1+t} = t - t^2 + t^3 - \cdots. \tag{10.4}$$

Therefore, near the critical point the divergent thermodynamical functions will display the same scaling behaviour as in (10.1) for the new scaling variable τ:

$$O(T) \approx A_O \tau^{-\rho}. \tag{10.5}$$

The scaling variables t and τ both become zero as the critical point is approached. However, they have very different high-temperature limits,

$$\lim_{T\to\infty} t = \infty, \tag{10.6}$$

$$\lim_{T\to\infty} \tau = 1. \tag{10.7}$$

From (10.6), the form (10.1) forces $O(T)$ to vanish in the high temperature limit. To accommodate a non-zero value for $O(T)$ in the limit, suppose that the amplitude A_O in (10.5) is extended to a temperature dependent amplitude, whose scaling behaviour is

$$\begin{aligned} O(T) \quad &\propto \quad O^*(T) \sim T^{\psi_O}(T - T_c)^{-\rho}, \\ &\sim \quad T^{\psi_O - \rho}\left(1 - \frac{T_c}{T}\right)^{-\rho}, \qquad (10.8) \\ &\sim \quad \beta^{\phi_O}\tau^{-\rho}. \qquad (10.9) \end{aligned}$$

where $\phi_O = \rho - \psi_O$. Taking limit of the above expression using (10.7) gives

$$\lim_{T\to\infty} O^*(T) \sim \beta^{\phi_O}. \tag{10.10}$$

Since the limit is non-zero, ϕ_O can be chosen to match the HTSE for O(T). Thus, from (10.9) the observable O(T) can be expressed as

$$O(T) = A_O O^*(T) = A_O \beta^{\phi_O} \tau^{-\rho} + \ldots, \tag{10.11}$$

where the dots represent higher-order corrections. The reduced magnetic susceptibility $\chi(T)/\beta$ is defined in (4.17). In the paramagnetic phase, $T > T_c$ and $\langle M \rangle = 0$ by definition. There,

$$\frac{\chi(T)}{\beta} = \frac{1}{N}\langle M^2 \rangle = \frac{1}{N}\sum_{i,j}\langle s_i s_j \rangle. \tag{10.12}$$

In the infinite temperature limit, the system is completely randomized; spins are up or down with no preferred direction. Thus, $\langle s_i s_j \rangle = 0$ if $i \neq j$. But if $i = j$, $\langle s_i s_j \rangle = \langle s_i^2 \rangle = 1$. Therefore, in the high-temperature limit, the reduced susceptibility approaches one.

$$\lim_{T\to\infty} \frac{\chi(T)}{\beta} = 1. \tag{10.13}$$

The HTSE for the reduced susceptibility is an expansion about high T or small β. This has the form

$$\chi(T)/\beta = a_0 + a_1\beta + a_2\beta^2 + a_3\beta^3 + \ldots. \tag{10.14}$$

Therefore, as temperature approaches infinity the expansion gives

$$\lim_{T\to\infty} \frac{\chi(T)}{\beta} = a_0. \tag{10.15}$$

Form (10.13), $a_0 = 1$ for all dimensions d. It can be said that $\phi_\chi = 0$ when the above expression is compared with (10.10). Thus this makes (10.5) a suitable expression to represent the susceptibility over broader temperature range. However, for the conventional scaling t the high temperature limit restricts the temperature scaling analysis to be close to the critical point.

The generic form for the susceptibility is known to be

$$\chi/\beta = At^{-\gamma}\left(1 + a_1 t^{\theta} + a_2 t^{2\theta} + \cdots + b_1 t + c_2 t^2 + \cdots\right) \tag{10.16}$$

there are two types of corrections. Those involving the universal exponent θ are called confluent corrections and the remaining correction are called analytic.

Two-Dimensional Case

For the two-dimensional case, the new scaling variable τ offers the scaling behaviour for the magnetic susceptibility as

$$\chi \approx A_\chi \tau^{-\gamma}. \tag{10.17}$$

where the critical exponent γ is known to be 7/4. In the vicinity of the critical point, the susceptibility for temperature greater than the critical temperature is expressed (Gartenhaus and McCullough 1988) as

$$\chi/\beta = C_0 t^{-7/4} + C_1 t^{-3/4} + D_0 + C_2 t^{1/4} + E_0 t \ln(t) + D_1 t + C_3 t^{5/4} + \cdots, \tag{10.18}$$

where the values for the above constants are known and are given in Gartenhaus and McCullough (1988) as $C_0 = 0.9625817322\ldots$, $C_1 = 0.074988\ldots$, $D_0 = -0.10413324511\ldots$, $C_2 = 0.147019\ldots$, $E_0 = 0.139942\ldots$, $D_1 = 0.0403255003\ldots$ and $C_3 = -0.14869\ldots$. Now using τ as the scaling variable instead of t, the critical expansion can be written as

$$\chi/\beta = C_0 \tau^{-7/4} + C_1' \tau^{-3/4} + D_0 + C_2' \tau^{1/4} + E_0 \tau \ln(\tau) + D_1 \tau + C_3' \tau^{5/4} + \cdots \tag{10.19}$$

where C_1', C_2' and C_3' are obtained by putting (10.3) into (10.18) and expanding.

Gofman *et al.* (1993) give the HTSE up to the fifteenth order in $\tanh(\beta)$ for d-dimensional Ising models. Converting this to a power series in β in two dimensions, one obtains

$$\begin{aligned}\chi/\beta \;=\; & 1 + 4\beta + 12\beta^2 + \frac{104}{3}\beta^3 + 92\beta^4 + \frac{3608}{15}\beta^5 + \frac{3056}{5}\beta^6 + \frac{484528}{315}\beta^7 + \frac{400012}{105}\beta^8 + \\ & \frac{26548808}{2835}\beta^9 + \frac{107828128}{4725}\beta^{10} + \frac{8625391648}{155925}\beta^{11} + \frac{6926560288}{51975}\beta^{12} + \\ & \frac{1945106545216}{6081075}\beta^{13} + \frac{10844734860976}{14189175}\beta^{14} + \frac{8130987171952}{4465125}\beta^{15} + \\ & O(\beta^{16}).\end{aligned} \tag{10.20}$$

This expansion is to fifteenth order. It was compared to the most recent HTSE for the $d = 2$ model in Butera and Comi (2002) and checked for consistency.

In terms of t and τ, β can be written

$$\beta = \frac{1}{T_c(1+t)} = \frac{1-\tau}{T_c}. \tag{10.21}$$

For the Ising model in two dimensions, the critical temperature on a square lattice is exactly known to be (Kramers and Wannier 1941)

$$T_c = \frac{2}{\ln(1+\sqrt{2})} = 2.269185\cdots. \tag{10.22}$$

Equations (10.20), (10.21) and (10.22) give the HTSE in terms of t and τ. While (10.18) and (10.19) give the critical expansion in terms of t and τ.

Now, in order to demonstrate and compare the behaviour of both the scaling variables, the susceptibility is plotted against $\ln(t)$ and $\ln(\tau)$ on the logarithmic scale following Campbell, Hukushima and Takayama (2006). Figures 10.1 and 10.2 depict the comparison of both the scalings using the HTSE and the critical analysis (see Appendix C for Maple Worksheet).

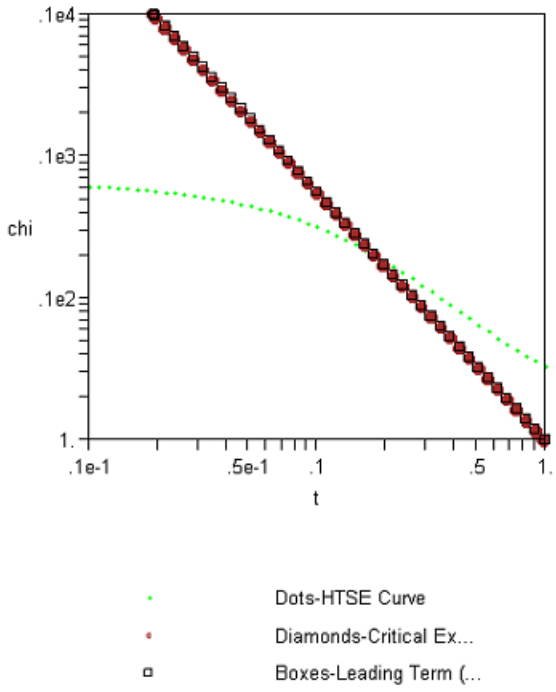

Figure 10.1: Susceptibility of the $d = 2$ Ising model as a function of t. The leading term $A_\chi t^{-\gamma}$ (boxes) follows the critical expansion (diamonds) for small t but misses the HTSE (points) at large t.

In Figure 10.1, the critical expansion is plotted in terms of t as in (10.18) along with the

HTSE also in terms of t (10.20). Following Campbell, Hukushima and Takayama (2006), the leading behaviour

$$A_\chi t^{-\gamma}.$$

is also depicted, with $A_\chi = 0.962581\cdots$ and $\gamma = 7/4$. It is clear that, while this curve overlaps with the critical expansion, it deviates from the HTSE for large enough t. This situation is usually considered as due to strong correction terms.

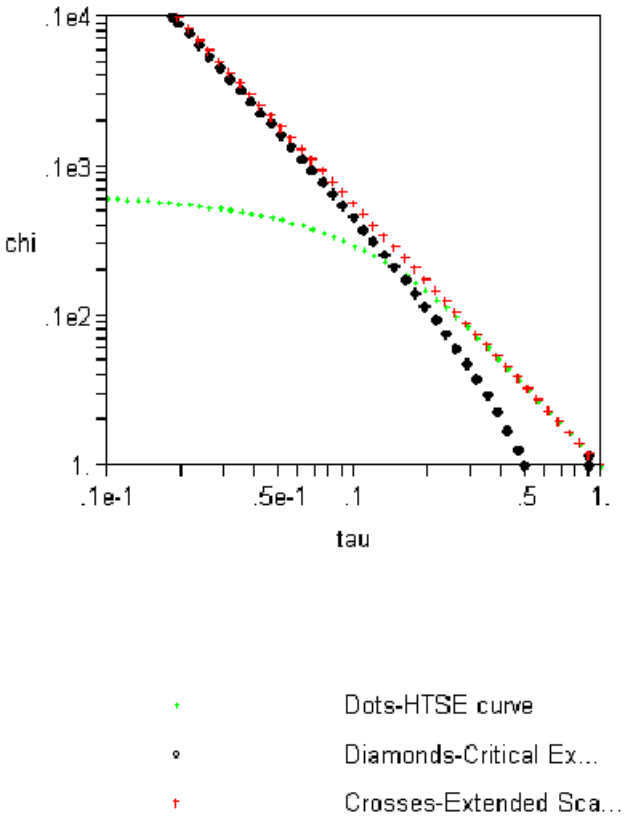

Figure 10.2: Susceptibility of the $d = 2$ Ising model as a function of τ. The extended scaling curve (crosses) follows the critical expansion (diamonds) for small τ and the HTSE (points) for large τ.

In Figure 10.2, the critical expansion is plotted in terms of τ as in (10.19) together with the HTSE (10.20) expressed in terms of τ. Again following Campbell, Hukushima and

Takayama (2006), these are compared with

$$A_\chi \tau^{-\gamma}.$$

Now, the τ curve follows the critical curve for small τ and switches to the HTSE for larger τ. In this manner, τ-scaling is claimed to be superior to t-scaling.

In the above scheme, A_χ in (10.17) was set to $0.96258\ldots$. Since $\tau \to 1$ as $T \to \infty$, (10.17) cannot satisfy (10.13). To remedy this, one may instead plot

$$\chi/\beta = A_\chi \tau^{-7/4} + C. \tag{10.23}$$

where $C = 1 - A_\chi$. In the $d = 2$ cases, $C = 0.03742$ and its inclusion would not be visible in figures 10.1 and 10.2. However, in the higher dimension and an analysis that follows, C is included in the extended scaling scheme (Berche *et al.* 2008).

Extended Scaling in High Dimensions

Now, above four dimensions, the leading scaling behaviour for the susceptibility comes from mean field theory (MFT) where γ takes the value 1. The critical expansion for $d = 5, 6, 7$ and 8 is given by Guttmann (1981):

$$\chi(T)/\beta = At^{-1} + Bt^{-\frac{1}{2}} + C + Dt^{\frac{1}{2}} + \ldots, \quad \text{for } d = 5, \tag{10.24}$$

$$\chi(T)/\beta = At^{-1} + B\ln t + C + Dt\ln t + \ldots, \quad \text{for } d = 6, \tag{10.25}$$

$$\chi(T)/\beta = At^{-1} + C + Dt^{\frac{1}{2}} + \ldots, \quad \text{for } d = 7, \tag{10.26}$$

$$\chi(T)/\beta = At^{-1} + C + Dt + \ldots, \quad \text{for } d = 8. \tag{10.27}$$

Guttmann (1981) with the help of series analysis technique examined corrections to scaling in dimensions five and six and also determined the critical temperatures and the amplitudes. In particular, Guttmann estimated $A = 1.311(9)$ and $B = -0.48(3)$ in five dimensions and $A = 1.168(8)$ in six dimensions. Since the corrections for $d = 6$ are logarithmic, it was not possible to measure the amplitudes in six dimensions using his

technique.

Next, using the new extended scaling method, the critical expansion for the five-dimensional case (10.24) is written as

$$\chi(T)/\beta = A\tau^{-1} + B\tau^{-\frac{1}{2}} + C(\tau), \tag{10.28}$$

where the higher order corrections are given by $C(\tau)$, which in the high-temperature regime goes to a constant C. Since both τ and $\chi(T)/\beta$ approach one, therefore the constant C equals $1 - A - B$. Similarly, the extended critical expansion for six is

$$\chi(T)/\beta \sim A\tau^{-1} + B\ln(\tau) + C, \tag{10.29}$$

and for higher (i.e, seven and eight) dimensions it is

$$\chi(T)/\beta \sim A\tau^{-1} + C. \tag{10.30}$$

where $C = 1 - A$.

Gofman *et al.* (1993) give the high temperature series expansion (HTSE) up to fifteenth order in $\tanh(\beta)$ for d-dimensional Ising models. Following this, Münkel *et al.* (1993) analyzed the HTSE for $d = 5$. The logarithmic term in six dimensions was also not explicitly handled in the series expansion approach of Gofman *et al.* (1993).

Next, in order to test the extended scaling scheme in five and six dimensions, the two scaling variables t and τ are plotted against χ on the logarithmic scale.

Five-Dimensional Case

In Figure 10.3, the critical expansion is plotted in terms of t as in (10.24) together with the HTSE (Gofman *et al.* 1993) which is

$$\begin{aligned}\chi/\beta &= 1 + 10\beta + 90\beta^2 + \frac{2420}{3}\beta^3 + 7150\beta^4 + \frac{190084}{3}\beta^5 + \\ &\quad \frac{1678172}{3}\beta^6 + \frac{311122568}{63}\beta^7 + \frac{304644370}{7}\beta^8 + \frac{217457614564}{567}\beta^9 +\end{aligned}$$

$$\frac{3190680657532}{945}\beta^{10} + \frac{926942841142568}{31185}\beta^{11} + \frac{1631038171336396}{6237}\beta^{12} + \frac{254381021406383608}{110565}\beta^{13} + \frac{193326245082386872}{9555}\beta^{14} + \frac{22722245900829817525936}{127702575}\beta^{15} + O(\beta^{16}). \quad (10.31)$$

In this case, the critical temperature T_c, known from the previous estimates, is 8.77844 (Luijten *et al.* 1999 and Aktekin *et al.* 1999). It is clear that, in the lower temperature limit both the curves are far away from each other (as the HTSE is inaccurate) and as the temperature increases the curves get closer and closer. However, at a certain temperature the critical expansion (which now becomes inaccurate) completely deviates from HTSE.

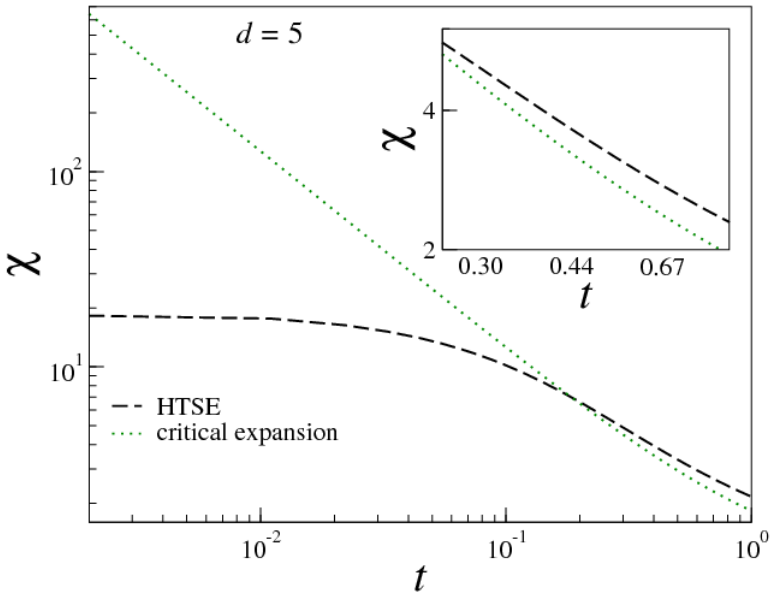

Figure 10.3: Five-Dimensional Ising model as a function of (t). The picture illustrates the deviation of the critical expansion (dots) from the HTSE (dashes).

On the other hand, in Figure 10.4, the extended critical expansion is plotted in terms of τ as in (10.28) along with the HTSE (Gofman *et al.* 1993) expressed in terms of τ and the critical expansion (Guttmann 1981). The extended scaling curve follows the critical curve and switches to the HTSE for high temperature ($\tau \to 1$). The figure shows that in high temperature regime the critical curve (Guttmann 1981) deviates from the extended critical expansion and the HTSE shifts away from the extended curve in the low temperature regime. However, the extended scaling curve follows the critical expansion and the

HTSE. Thus, it is clear that the extended scaling scheme is superior than the conventional scheme in high dimensions. However, in order to build confidence in this approach, the testing was next done in dimension six.

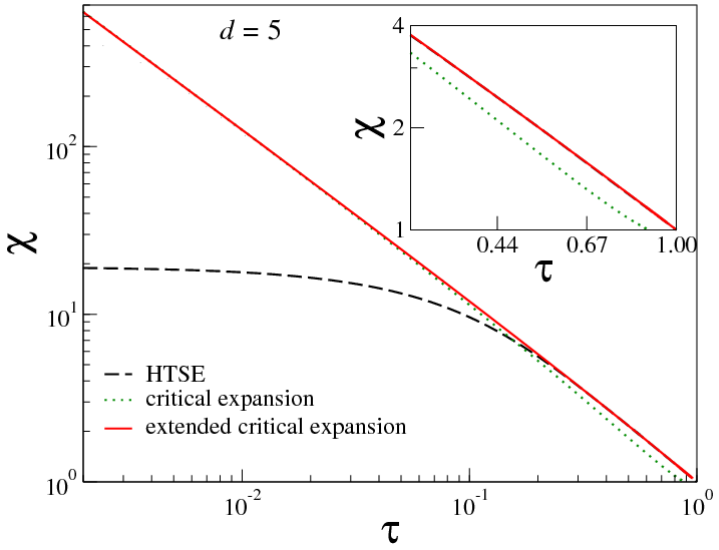

Figure 10.4: Five-Dimensional Ising model as a function of (τ). The extended critical expansion (line) follows the critical expansion (dots) for small τ and the HTSE (dashes) for large τ.

Six-Dimensional Case

In Figure 10.5, on the logarithmic scale the critical expansion (10.25) and HTSE (Gofman *et al* 1993) in terms of t are plotted. In this case, the critical temperature T_c, measured by Gofmann *et al.* (1993), is 10.8348(4) and the HTSE is

$$\begin{aligned}\chi/\beta &= 1+12\beta+132\beta^2+1448\beta^3+15764\beta^4+\frac{858008}{5}\beta^5+\\ &\frac{27958288}{15}\beta^6+\frac{2125714096}{105}\beta^7+\frac{23067124964}{105}\beta^8+\frac{2252809008008}{945}\beta^9+\\ &\frac{17453066574784}{675}\beta^{10}+\frac{14575983595475296}{51975}\beta^{11}+\frac{43103828200446848}{14175}\beta^{12}+\\ &\frac{66834599442777894016}{2027025}\beta^{13}+\frac{5071868185418360071376}{14189175}\beta^{14}+\end{aligned}$$

$$\frac{8247605149552033062309 92}{212837625}\beta^{15} + O(\beta^{16}). \tag{10.32}$$

As in the five-dimensional case, figure 10.5 illustrates the deviation of critical expansion from the HTSE in the high temperature limit.

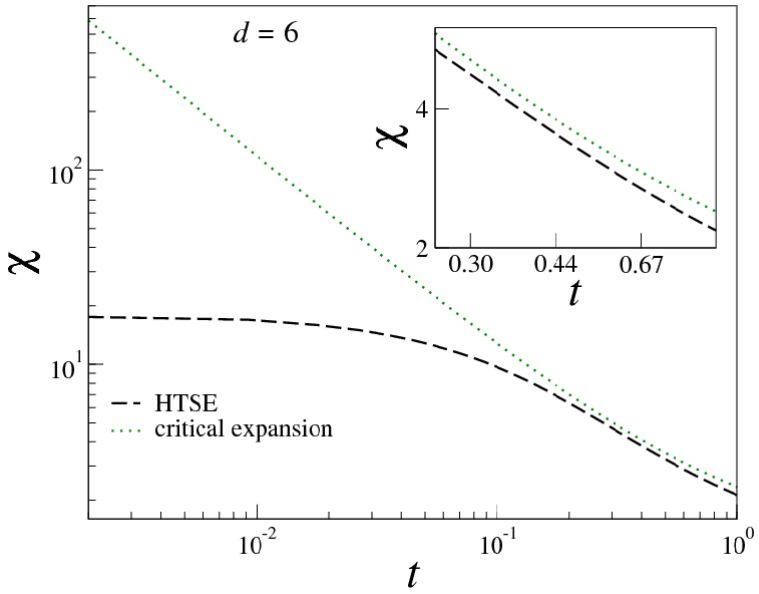

Figure 10.5: Six-Dimensional Ising model in terms of (t). The inset exhibits the deviation of critical expansion (dots) form the HTSE (dashes).

Figure 10.6 exhibits the extended critical curve (10.29) where $A_\chi = 1.168(8)$ together with the HTSE and the critical curve in terms τ. It is clear from the figure that the extended curve coincides with the critical and the HTSE curve in the regions where they are valid. As in $d = 5$, the critical curve and HTSE for six dimensions deviates from the extended critical curve when theirs an increase and decrease in temperature. In the same manner, it is clear that the extended scaling method is more powerful than the standard reduced temperature, respectively. Thus, the confidence has now been build up in the new approach and the analysis for seven and eight dimensions can be carried out only using the extended scaling approach.

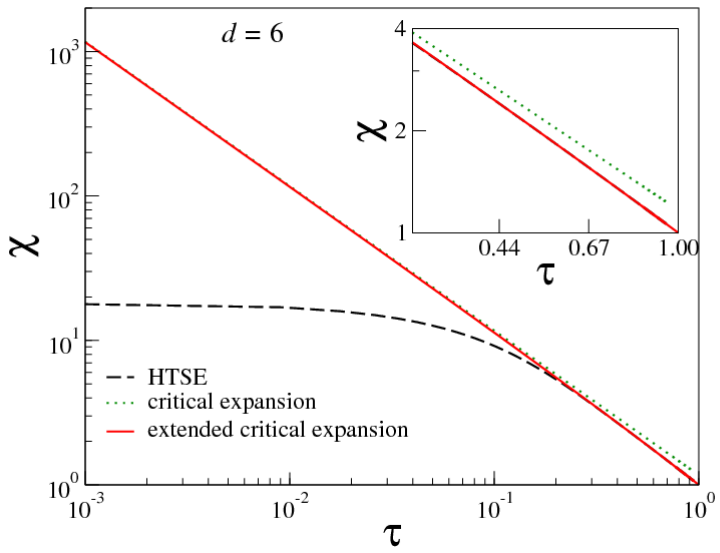

Figure 10.6: Six-Dimensional Ising model in terms of (τ). The extended scaling curve (line) coincides with the HTSE (dashes) and the critical expansion (dots).

Now that extended scaling is shown to be better than the t, one can apply this technique to higher dimensions to measure critical temperature and the amplitudes. In particular, a computational method was used to generate points which corresponds to the HTSE. Best fits were performed to equation (10.28), (10.29) and (10.30). While this procedure lies outside the remit of this project, the results are summarized (Table 10.1) here for completeness and the reader is referred to Berche *et al.* (2008).

Seven-Eight Dimensional Case

For the seven-eight dimensional case, the extended critical expansion as in (10.30) and the HTSE (Gofmann *et al.* 1993) as function of τ, given by,

$$\begin{aligned}\chi/\beta &= 1 + 14\beta + 182\beta^2 + \frac{7084}{3}\beta^3 + \frac{91406}{3}\beta^4 + \frac{5896828}{15}\beta^5 + \\ &\frac{227931844}{45}\beta^6 + \frac{2936779784}{45}\beta^7 + \frac{37818523538}{45}\beta^8 + \frac{4383097815604}{405}\beta^9 + \\ &\frac{282145777215532}{2025}\beta^{10} + \frac{39956654372229944}{22275}\beta^{11} + \frac{1543020715401325036}{66825}\beta^{12} +\end{aligned}$$

Table 10.1: Summary of the computational results recently obtained by Berche *et al.* (2008).

$$\frac{23473837517766645928}{78975}\beta^{13} + \frac{1789600002676293361688}{467775}\beta^{14} + \frac{44917467526640899711070 08}{91216125}\beta^{15} + O(\beta^{16}). \tag{10.33}$$

are plotted against the susceptibility on the logarithmic scale. The critical amplitude and the critical temperature are known from the recent analysis by Berche *et al.* (2008) for seven as $A = 1.1008(5)$, $C = -0.1008(5)$, $T_c = 12.8690(3)$ and $\gamma = 1.000(2)$ and eight dimensions as $A = 1.0836(5)$, $C = -0.0836(5)$, $T_c = 14.8933(8)$ and $\gamma = 0.998(2)$. The inset in the figure 10.7 and 10.8 illustrates the cross over of the extended critical curve and the HTSE in the high temperature. However, at low temperature the extended curve deviates from the HTSE. This simulation shows the perfectness of the variable τ.

It would be interesting to apply this technique to other spin models such as discussed in section 6.

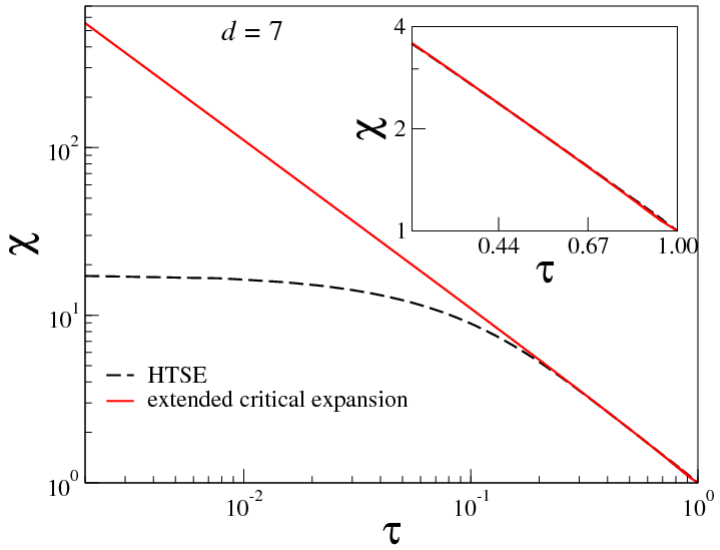

Figure 10.7: Seven-Dimensional Ising model as a function of (τ). The figure illustrates the cross over of the extended critical expansion (line) and the HTSE (dashes).

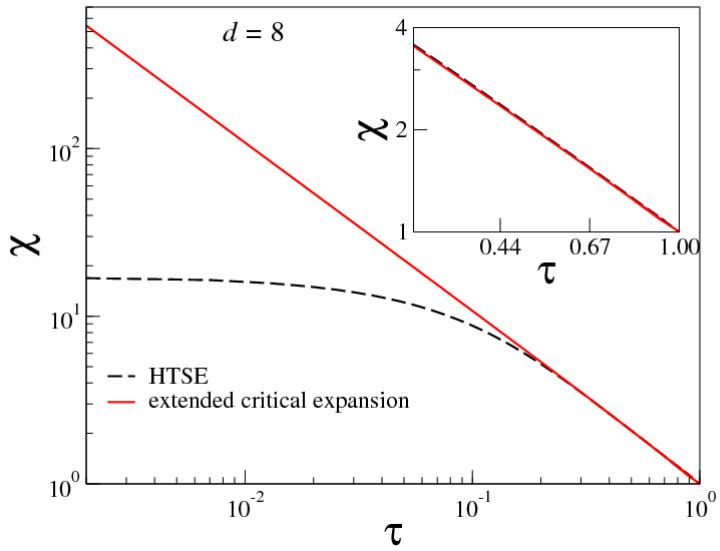

Figure 10.8: Eight-Dimensional Ising model as (τ) scaling variable. The inset shows the cross over of extended expansion (line) and the high temperature expansion (dashes).

11 Conclusion

In this project, an introduction to statistical mechanics was given. The Ising model of phase transitions was then introduced and different types of transitions discussed. Continuous phase transitions are described by six critical exponents. These are, however, not all independent, instead they are linked through the scaling relations, which were also derived. Re-derivations of the one-dimensional Ising model and MF theory were then performed and the scaling relations were seen to be satisfied.

On the basis of the rationale given by the Campbell, Hukushima and Takayama (2006), the new extended scaling method was retested in two-dimensional Ising model and shown to be superior to the conventional scaling approach. Extended scaling was than tested and applied above the upper critical dimensions i.e., for $d > 4$. The suitability of this approach in five and above dimensions was shown. The qualitative results presented herein formed the basis for a more quantitative collaborative work which has now been published (Berche *et al.* 2008) and here presented in Appendix D.

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A Appendix

The Relationship between Magnetisation and the Free Energy

Following is the derivation of the relationship (4.16). Differentiating the free energy (4.15) with respect to reduced external field h gives

$$\frac{\partial f}{\partial h} = \frac{-kT}{N}\frac{1}{Z}\frac{\partial Z}{\partial h}. \tag{A.1}$$

The first derivative of the partition function (4.14) with respect to h is

$$\frac{\partial Z}{\partial h} = \sum_{\{s_i\}} e^{-\beta E + hM} M, \tag{A.2}$$

and the expectation value of the total magnetisation is

$$\langle M \rangle = \frac{1}{Z}\sum_{\{s_i\}} e^{-\beta E + hM} M. \tag{A.3}$$

Thus, using (A.2), (A.3) and (4.8), the expression (A.1) can be expressed as

$$\frac{\partial f}{\partial h} = -kT\frac{\langle M \rangle}{N}, \tag{A.4}$$

$$= -kTm. \tag{A.5}$$

Next differentiating the reduced field (4.13) with respect to H gives

$$\frac{\partial h}{\partial H} = \beta. \tag{A.6}$$

Multiplying (A.5) and (A.6) yields

$$\frac{\partial f}{\partial h}\frac{\partial h}{\partial H} = -m. \tag{A.7}$$

Therefore, the above expression gives the relationship (4.16), which is the first derivative of the free energy with respect to H.

$$m = -\frac{\partial f}{\partial h}\frac{\partial h}{\partial H} = -\frac{\partial f}{\partial H}. \tag{A.8}$$

The Relationship Between Susceptibility and the Free Energy

Now, differentiating the free energy twice with respect to reduced external field yields

$$\begin{aligned} \frac{\partial^2 f}{\partial h^2} &= \frac{1}{N}\frac{\partial^2(\ln Z)}{\partial h^2}, \\ &= \frac{1}{N}\frac{\partial}{\partial h}\left[\frac{1}{Z}\frac{\partial Z}{\partial h}\right]. \end{aligned} \tag{A.9}$$

Altering the differential term in the above equation gives the free energy to

$$\begin{aligned} \frac{\partial^2 f}{\partial h^2} &= \frac{1}{N}\frac{\partial}{\partial h}(Z^{-1}Z'), \\ &= \frac{1}{N}[-Z^{-2}Z'Z' + Z^{-1}Z''], \\ &= \frac{1}{N}\left[\frac{1}{Z}\frac{\partial^2 Z}{\partial h^2} - \left(\frac{1}{Z}\frac{\partial Z}{\partial h}\right)^2\right]. \end{aligned} \tag{A.10}$$

Differentiating (A.2) again gives

$$\frac{\partial^2 Z}{\partial h^2} = \sum_{\{s_i\}} M^2 e^{-\beta E + hM}. \tag{A.11}$$

Substituting (A.2) and (A.11) into (A.10) and using (A.3) gives

$$\frac{\partial^2 f}{\partial h^2} = \frac{1}{N}[\left\langle M^2 \right\rangle - \langle M \rangle^2] \tag{A.12}$$

Now, manipulating the expression in (4.17) gives

$$\chi = \frac{1}{N}\left\langle (\langle M \rangle - M)^2 \right\rangle, \tag{A.13}$$

$$\begin{aligned} &= \frac{1}{N}\left\langle \langle M \rangle^2 - 2\langle M \rangle M + M^2 \right\rangle, \\ &= \frac{1}{N}\left[\left\langle \langle M \rangle^2 \right\rangle - 2\langle M \rangle \langle M \rangle + \left\langle M^2 \right\rangle\right], \\ &= \frac{1}{N}\left[-\langle M \rangle^2 + \left\langle M^2 \right\rangle\right]. \end{aligned} \tag{A.14}$$

Thus, comparing this with (A.12) yields that susceptibility equals the second derivative of the free energy;

$$\chi = \frac{\partial^2 f}{\partial h^2}. \tag{A.15}$$

The Relationship Between the Internal Energy and the Free Energy

Since, the internal energy is the first derivative of the free energy, in terms of β. Therefore, it is written as

$$\frac{\partial f}{\partial \beta} = \frac{1}{N}\frac{1}{Z}\frac{\partial Z}{\partial \beta}, \tag{A.16}$$

The differential term in the above expression can be simplified to give

$$\frac{\partial f}{\partial \beta} = \frac{1}{N}\frac{1}{Z}\sum_{\{s_i\}}(-E)e^{-\beta E+hM}. \tag{A.17}$$

However, the expectation value of the energy is

$$\langle E\rangle = \frac{1}{Z}\sum_{\{s_i\}}(-E)e^{-\beta E+hM}. \tag{A.18}$$

Substituting the above expression in (A.17) yields

$$\frac{\partial f}{\partial \beta} = e. \tag{A.19}$$

Hence, the above result gives another relationship of thermodynamic quantities.

The Relationship Between Specific Heat and the Free Energy

In order to prove the specific heat and the free energy relation, differentiate twice the free energy with respect to β.

$$\frac{\partial^2 f}{\partial \beta^2} = \frac{1}{N}\frac{\partial}{\partial \beta}\left[\frac{1}{Z}\frac{\partial Z}{\partial \beta}\right]. \tag{A.20}$$

Differentiating further gives

$$\begin{aligned}\frac{\partial^2 f}{\partial \beta^2} &= \frac{1}{N}\frac{\partial}{\partial \beta}(Z^{-1}Z'),\\ &= \frac{1}{N}(-Z^{-2}Z'' + Z^{-1}Z''),\\ &= \frac{1}{N}\left(\frac{1}{Z}\frac{\partial^2 Z}{\partial \beta^2} - \left(\frac{1}{Z}\frac{\partial Z}{\partial \beta}\right)^2\right).\end{aligned} \tag{A.21}$$

From (4.15), the first and the second derivative of the free energy can be found. Therefore, substituting these derivatives results

$$\frac{\partial^2 f}{\partial \beta^2} = \frac{1}{N}\left(\left\langle E^2 \right\rangle - \langle E \rangle^2\right). \tag{A.22}$$

The internal energy is the variance of the energies and rearranging this energy gives

$$\begin{aligned} C &= \frac{1}{N}\left\langle (E - \langle E \rangle)^2 \right\rangle, && \text{(A.23)} \\ &= \frac{1}{N}\left[\left\langle E^2 - 2E\langle E \rangle + \langle E \rangle^2 \right\rangle\right], \\ &= \frac{1}{N}\left[\left\langle E^2 \right\rangle - \langle 2E\langle E \rangle \rangle + \left\langle \langle E \rangle^2 \right\rangle\right], \\ &= \frac{1}{N}\left[\left\langle E^2 \right\rangle - \langle E \rangle^2\right]. && \text{(A.24)} \end{aligned}$$

Thus, comparing these results with (A.22) yields the wanted relationship which is

$$\frac{\partial^2 f}{\partial \beta^2} = C. \tag{A.25}$$

B Appendix

Derivation of the Gaussian Identity

Consider

$$I = \int_{\infty}^{\infty} e^{-ax^2+bx+c} dx. \tag{B.1}$$

Manipulating the above expression gives

$$\begin{aligned} I &= \int_{\infty}^{\infty} e^{-\left(\sqrt{a}x - \frac{b}{2\sqrt{a}}\right)^2 + \frac{b^2}{4a} + c} dx, \\ &= e^{\frac{b^2}{4a}+c} \int_{\infty}^{\infty} e^{-\left(\sqrt{a}x - \frac{b}{2\sqrt{a}}\right)^2} dx. \end{aligned} \tag{B.2}$$

Let $\sqrt{a}x - \frac{b}{2\sqrt{a}} = y$, differentiating y gives

$$dx = \frac{1}{\sqrt{a}} dy. \tag{B.3}$$

Substituting the value for dx in (B.2) gives

$$I = e^{\frac{b^2}{4a}+c} \int_{\infty}^{\infty} e^{-y^2} \frac{1}{\sqrt{a}} dy. \tag{B.4}$$

Using the polar coordinates y change to r, the integral becomes

$$\begin{aligned} I &= e^{\frac{b^2}{4a}+c} \frac{1}{\sqrt{a}} \sqrt{\int_0^{2\pi} \int_0^{\infty} e^{-r^2} r dr d\theta}, \\ &= e^{\frac{b^2}{4a}+c} \frac{1}{\sqrt{a}} \sqrt{2\pi \left[-\frac{1}{2} e^{-r^2}\right]_0^{\infty}}, \\ &= e^{\frac{b^2}{4a}+c} \sqrt{\frac{\pi}{a}}. \end{aligned} \tag{B.5}$$

From (B.1) and (B.5), the gaussian identity is obtained.

$$\int_{\infty}^{\infty} e^{-ax^2+bx+c} dx = e^{\frac{b^2}{4a}+c} \sqrt{\frac{\pi}{a}}. \tag{B.6}$$